Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAVXR1614

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC 01	ChemPort single article sales feature unavailable
NEWS	3	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS	4	APR 07	STN is raising the limits on saved answers
NEWS	5	APR 24	CA/CAplus now has more comprehensive patent assignee information
NEWS	6	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS	7	APR 28	CAS patent authority coverage expanded
NEWS	8	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS	9	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS	10	MAY 08	STN Express, Version 8.4, now available
NEWS	11	MAY 11	STN on the Web enhanced
NEWS	12	MAY 11	BEILSTEIN substance information now available on STN Easy
NEWS	13	MAY 14	DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
NEWS	14	MAY 15	INPADOCDB and INPAFAMDB enhanced with Chinese legal status data
NEWS	15	MAY 28	CAS databases on STN enhanced with NANO super role in records back to 1992
NEWS	16	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:54:15 ON 17 JUN 2009

=> file registry
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.22 | 0.22

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 17 JUN 2009

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 JUN 2009 HIGHEST RN 1158168-92-3
DICTIONARY FILE UPDATES: 15 JUN 2009 HIGHEST RN 1158168-92-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

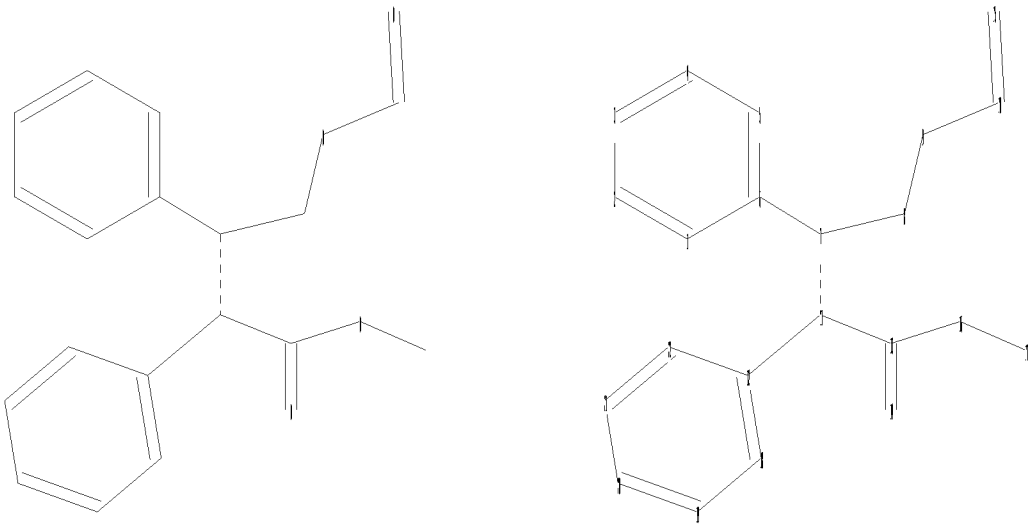
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red Folder\10586573\L1.str



chain nodes :
7 8 9 10 11 13 14 15 16 17
ring nodes :
1 2 3 4 5 6 12 18 19 20 21 22
chain bonds :
6-7 7-8 7-11 8-9 9-10 10-15 11-12 11-13 13-14 13-16 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-22 18-19 19-20 20-21 21-22

```
exact/norm bonds :
7-11  8-9  9-10  10-15  13-14  13-16  16-17
exact bonds :
6-7  7-8  11-12  11-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-18  12-22  18-19  19-20  20-21  21-22
isolated ring systems :
containing 1 : 12 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
 11:CLASS  12:Atom  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:Atom
19:Atom  20:Atom  21:Atom  22:Atom



L1      STRUCTURE UPLOADED

=> s sam sss l1
SAMPLE SEARCH INITIATED 10:55:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       29 TO ITERATE

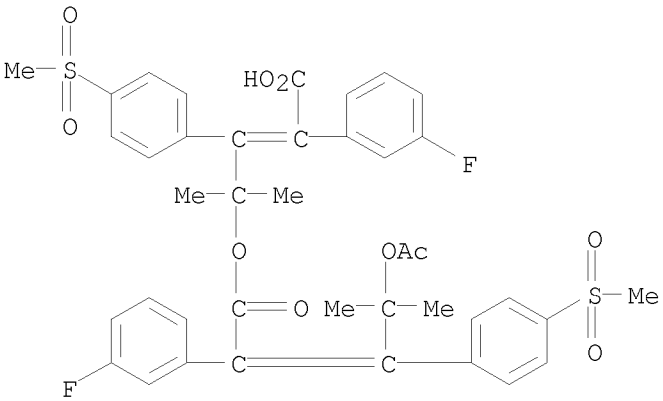
100.0% PROCESSED       29 ITERATIONS                                4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          257 TO      903
PROJECTED ANSWERS:               4 TO      200

L2            4 SEA SSS SAM L1

=> d sca

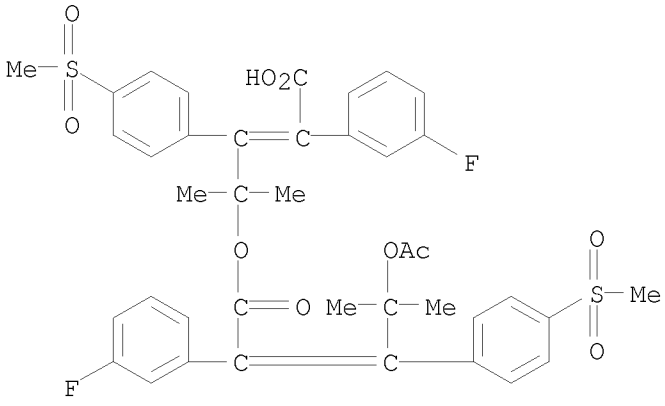
L2   4 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-
     3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-
     (methylsulfonyl)phenyl]propylidene]-3-fluoro-, sodium salt (1:1)
MF   C40 H38 F2 O10 S2 . Na
```



● Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-
MF C40 H38 F2 O10 S2
CI COM

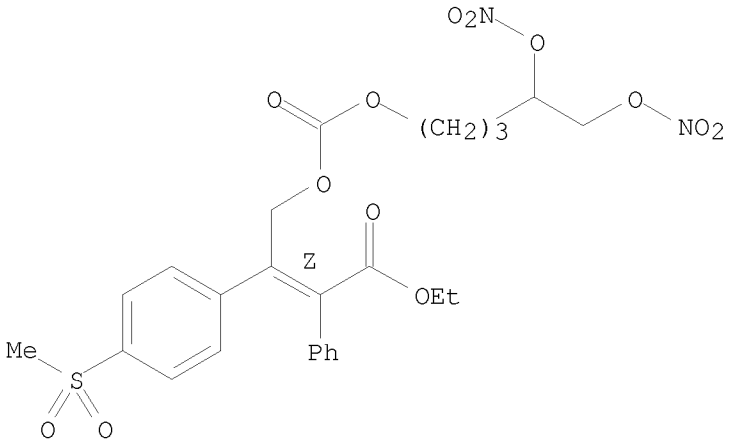


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)-
MF C25 H28 N2 O13 S

Double bond geometry as shown.

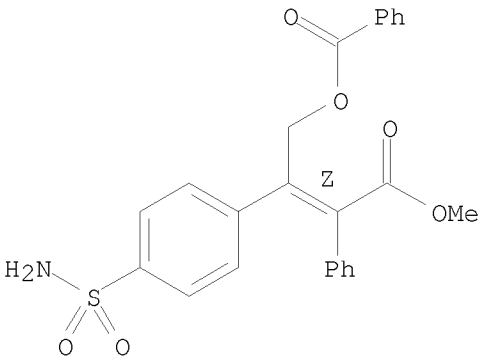


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(aminosulfonyl)phenyl]-2-(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI)
MF C24 H21 N O6 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

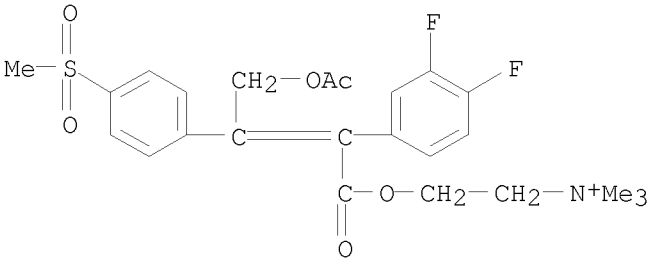
=> s full sss l1
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 11:12:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 767 TO ITERATE

100.0% PROCESSED 767 ITERATIONS 84 ANSWERS
SEARCH TIME: 00.00.01

L3 84 SEA SSS FUL L1

=> d sca

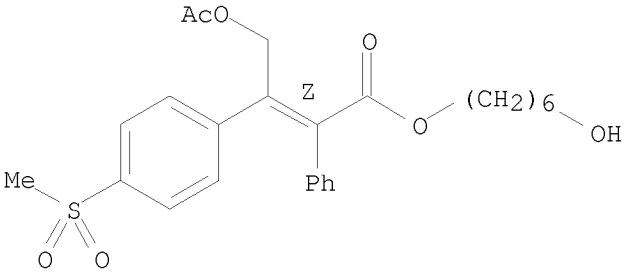
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-
MF C24 H28 F2 N O6 S
CI COM



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (αZ)-
MF C25 H30 O7 S

Double bond geometry as shown.

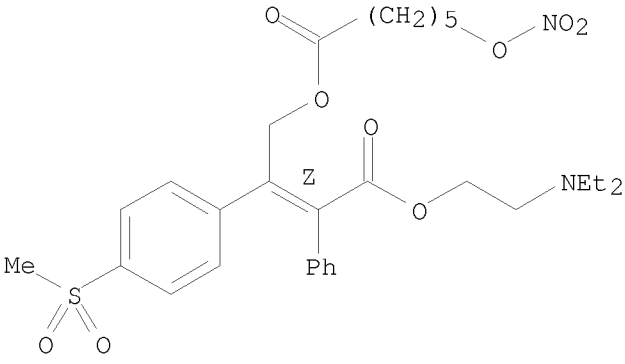


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, (αZ)-
MF C29 H38 N2 O9 S

Double bond geometry as shown.

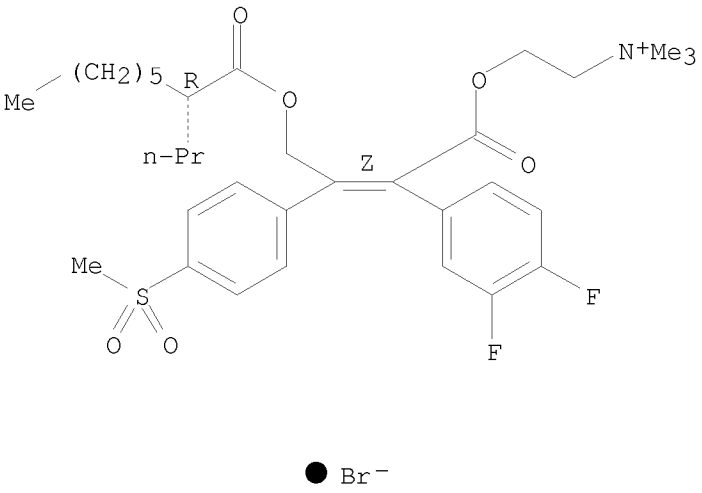


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-4-[[(2R)-1-oxo-2-propyloctyl]oxy]-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
MF C33 H46 F2 N O6 S . Br

Absolute stereochemistry.
Double bond geometry as shown.

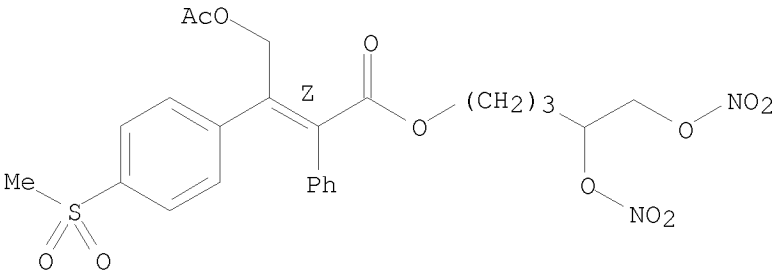


● Br^-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, (αZ)-
MF C24 H26 N2 O12 S

Double bond geometry as shown.

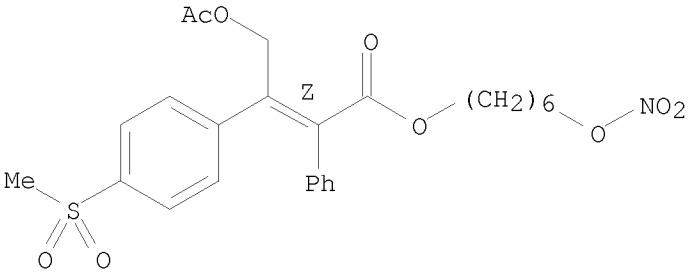


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
    (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (αZ)-
MF C25 H29 N O9 S

Double bond geometry as shown.

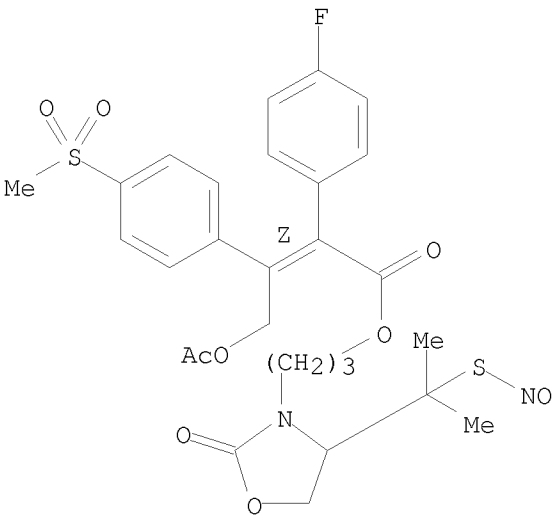


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
    (methylsulfonyl)phenyl]ethylidene]-4-fluoro-,
    3-[4-[1-methyl-1-(nitrosothio)ethyl]-2-oxo-3-oxazolidinyl]propyl ester,
    (αZ)-
MF C28 H31 F N2 O9 S2

Double bond geometry as shown.

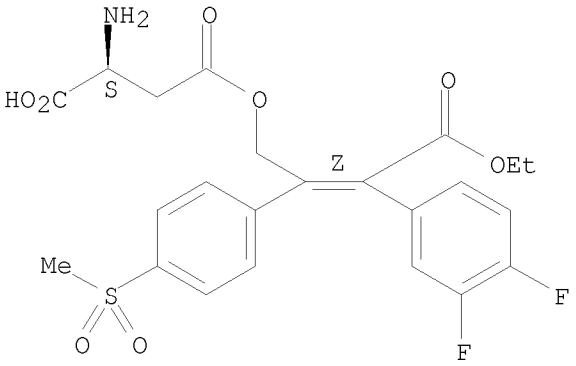


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN L-Aspartic acid, 4-[(2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester
MF C23 H23 F2 N O8 S

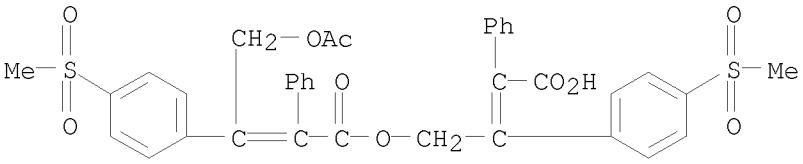
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester
MF C36 H32 O10 S2
CI COM

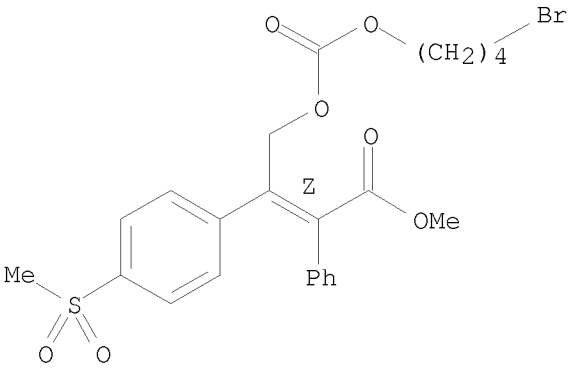


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)-
MF C23 H25 Br O7 S

Double bond geometry as shown.

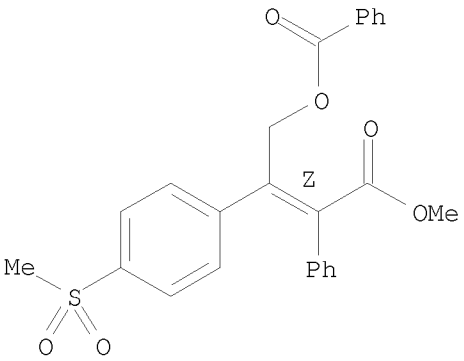


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(benzoyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI)
MF C25 H22 O6 S

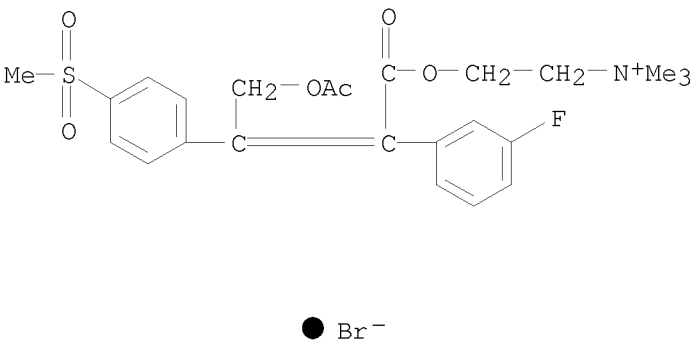
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

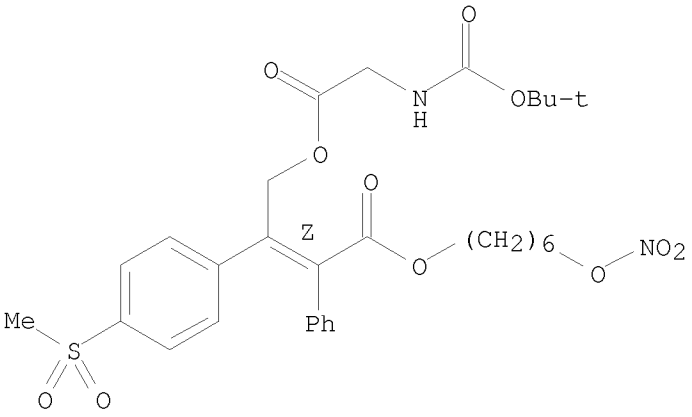
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
MF C24 H29 F N O6 S . Br



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester
MF C30 H38 N2 O11 S

Double bond geometry as shown.

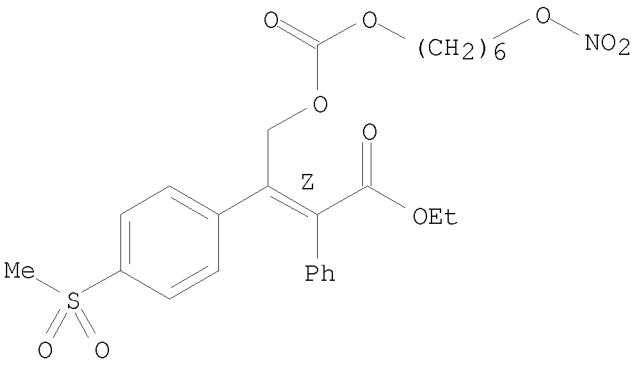


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, ethyl ester, (αZ)-
MF C26 H31 N O10 S

Double bond geometry as shown.

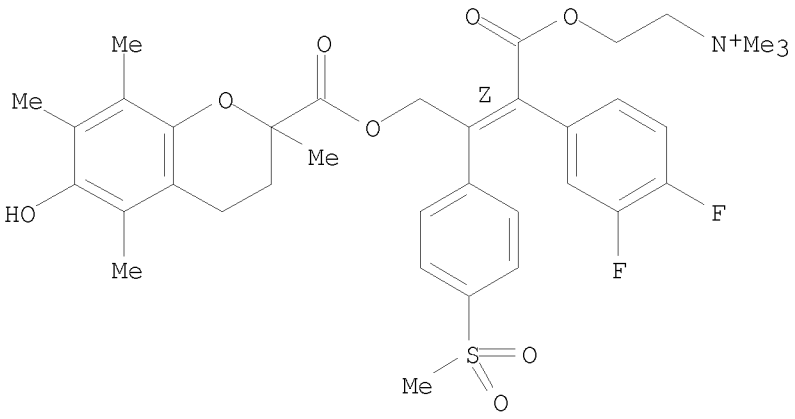


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-4-[[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)carbonyl]oxy]-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-
MF C36 H42 F2 N O8 S

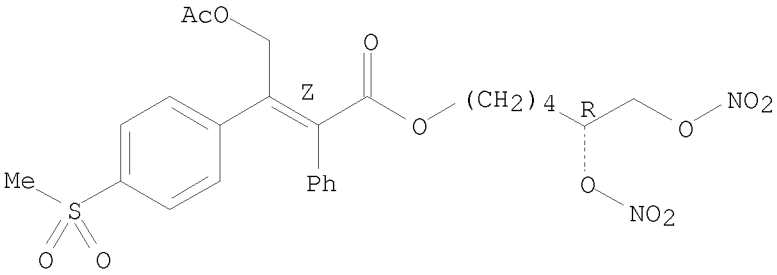
Double bond geometry as shown.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (αZ)-
MF C25 H28 N2 O12 S

Absolute stereochemistry.
Double bond geometry as shown.

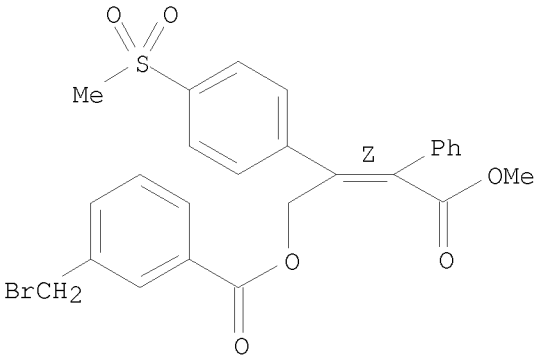


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[3-(bromomethyl)benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)-
MF C26 H23 Br O6 S

Double bond geometry as shown.

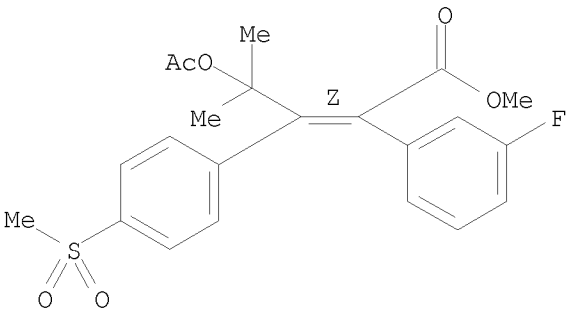


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, methyl ester, (αZ)-
MF C22 H23 F O6 S

Double bond geometry as shown.



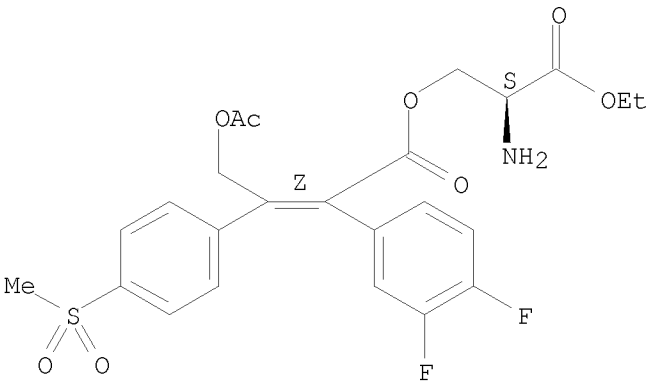
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

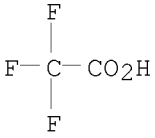
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (αZ)-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, 2,2,2-trifluoroacetate (1:1)
MF C24 H25 F2 N O8 S . C2 H F3 O2

CM 1

Absolute stereochemistry.
Double bond geometry as shown.

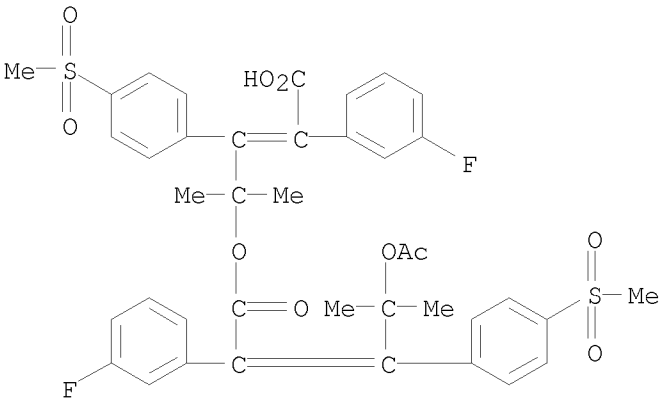


CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, sodium salt (1:1)
MF C40 H38 F2 O10 S2 . Na

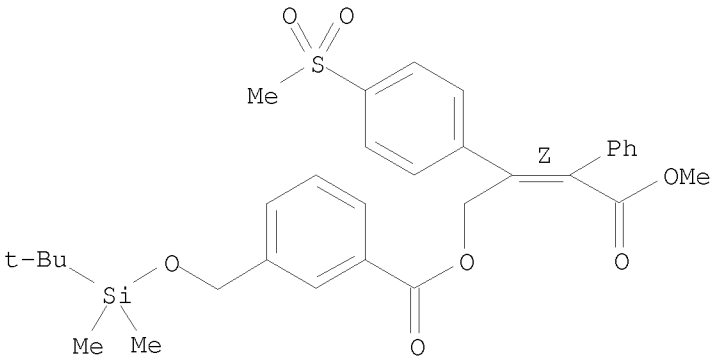


● Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)-
MF C32 H38 O7 S Si

Double bond geometry as shown.

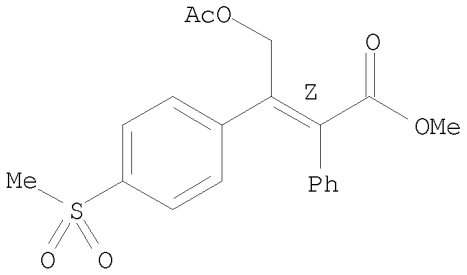


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI)
MF C20 H20 O6 S

Double bond geometry as shown.

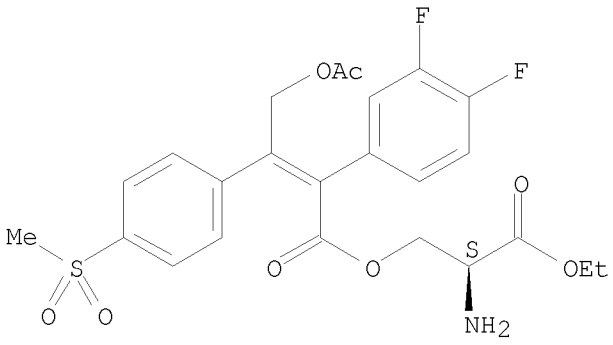


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester
MF C24 H25 F2 N O8 S

Absolute stereochemistry.
Double bond geometry unknown.

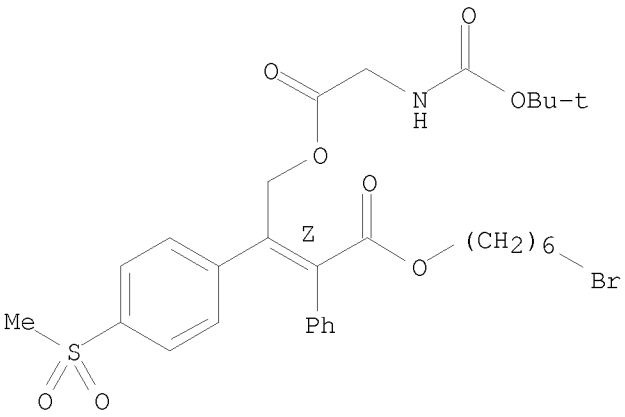


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-,
    (2Z)-4-[(6-bromohexyl)oxy]-2-[4-(methylsulfonyl)phenyl]-4-oxo-3-phenyl-2-
    buten-1-yl ester
MF C30 H38 Br N O8 S

Double bond geometry as shown.

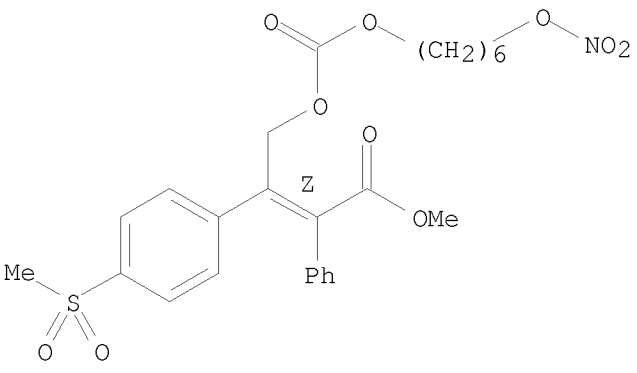


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[6-
    (nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (αZ)-
MF C25 H29 N O10 S

Double bond geometry as shown.

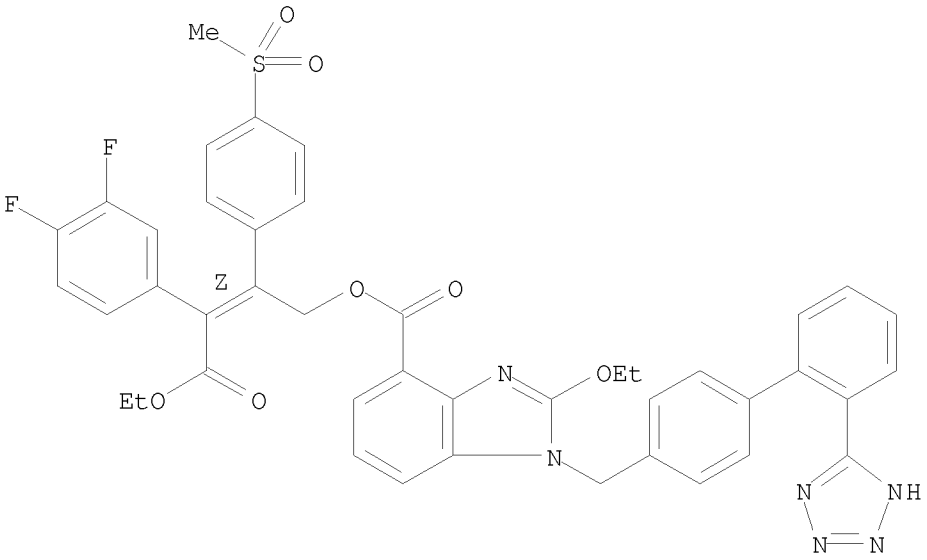


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Benzimidazole-4-carboxylic acid, 2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl ester
MF C43 H36 F2 N6 O7 S

Double bond geometry as shown.

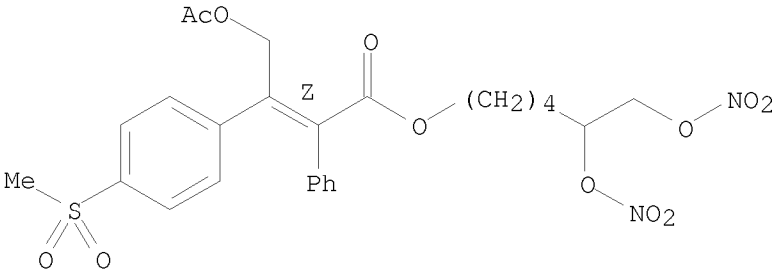


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)-
MF C25 H28 N2 O12 S

Double bond geometry as shown.

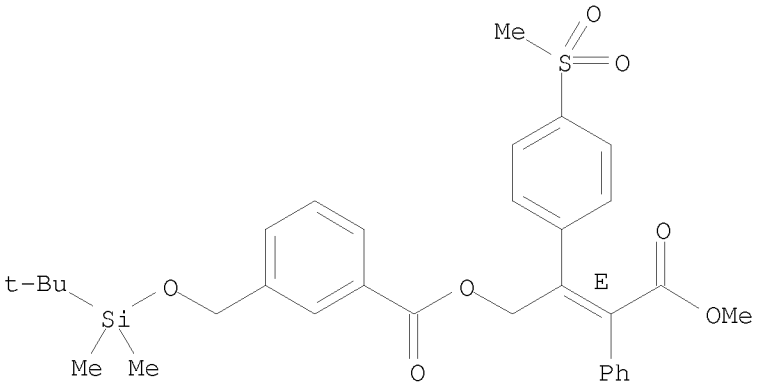


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αE)-
MF C32 H38 O7 S Si

Double bond geometry as shown.

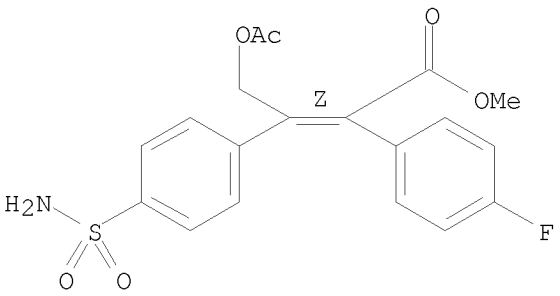


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI)
MF C19 H18 F N O6 S

Double bond geometry as shown.

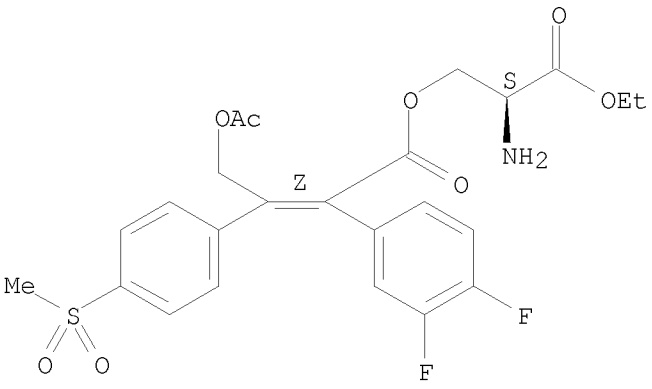


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, (αZ)-
MF C24 H25 F2 N O8 S
CI COM

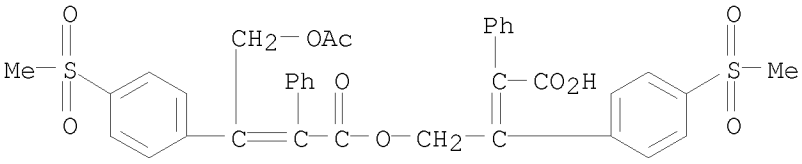
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

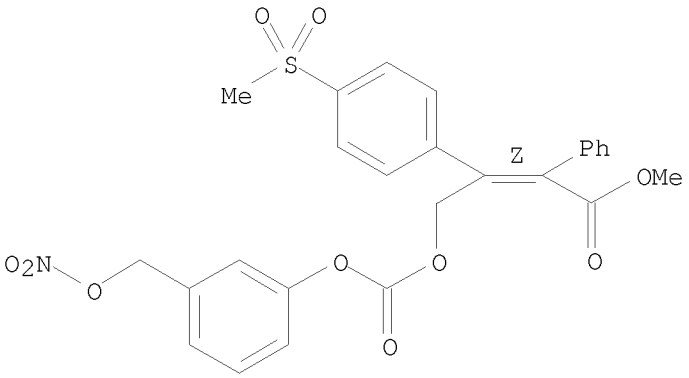
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester, sodium salt (1:1)
MF C36 H32 O10 S2 . Na



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[3-[(nitrooxy)methyl]phenoxy]carbonyl]oxy]ethylidene]-, methyl ester, (αZ)-
MF C26 H23 N O10 S

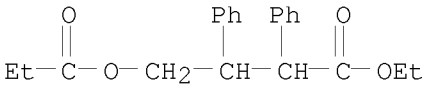
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

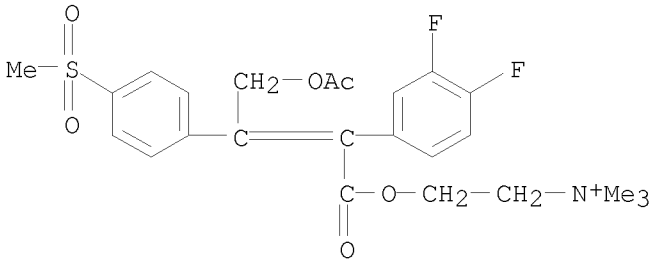
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzenepropanoic acid, β-[(1-oxopropoxy)methyl]-α-phenyl-, ethyl ester
MF C21 H24 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

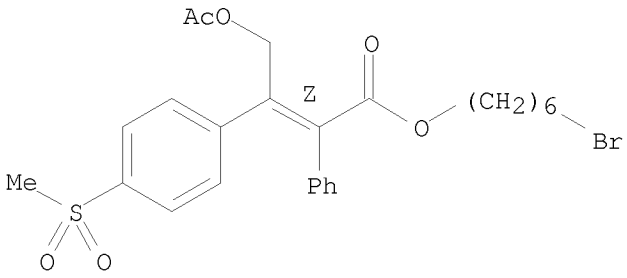
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
MF C24 H28 F2 N O6 S . Br



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (αZ)-
MF C25 H29 Br O6 S

Double bond geometry as shown.



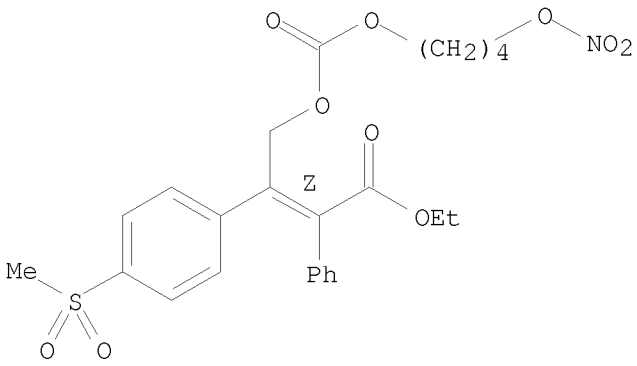
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, ethyl ester, (αZ)-

MF C24 H27 N O10 S

Double bond geometry as shown.

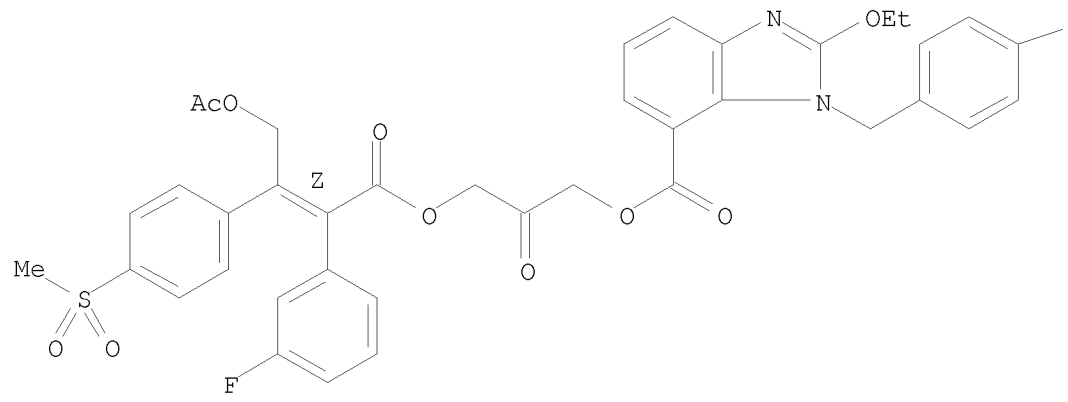


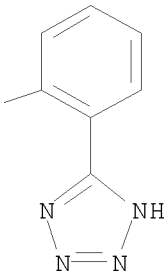
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Benzimidazole-7-carboxylic acid,
2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-,
3-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-2-oxopropyl ester
MF C46 H39 F N6 O10 S

Double bond geometry as shown.



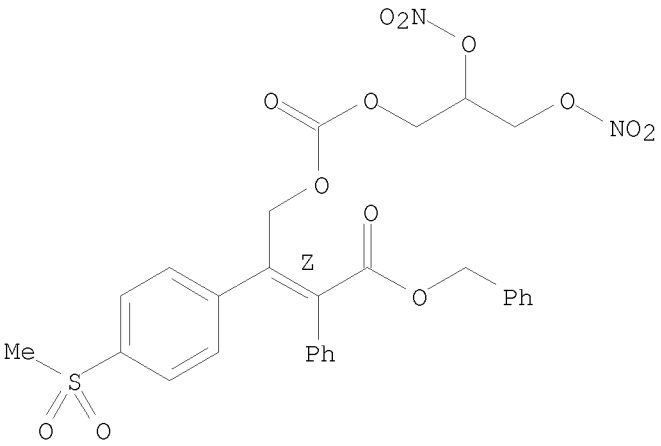


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, phenylmethyl ester, (αZ)-
MF C28 H26 N2 O13 S

Double bond geometry as shown.

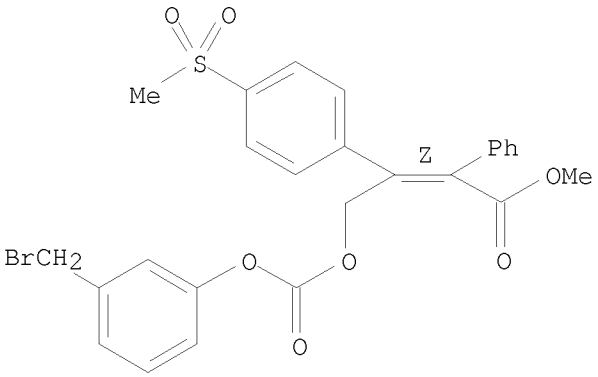


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[3-(bromomethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)-
MF C26 H23 Br O7 S

Double bond geometry as shown.

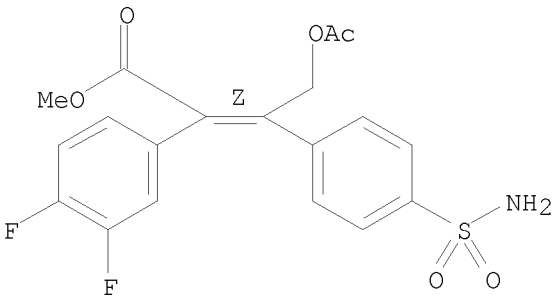


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI)
MF C19 H17 F2 N O6 S

Double bond geometry as shown.

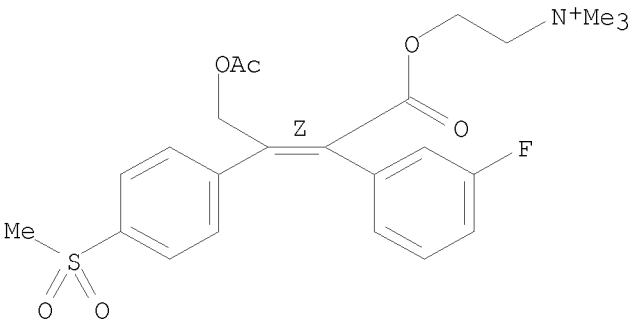


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

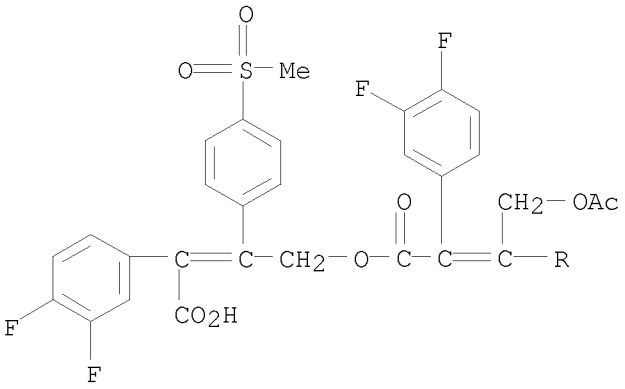
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-
MF C24 H29 F N O6 S
CI COM

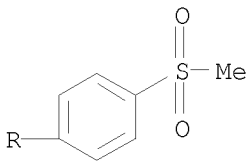
Double bond geometry as shown.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-
MF C36 H28 F4 O10 S2
CI COM





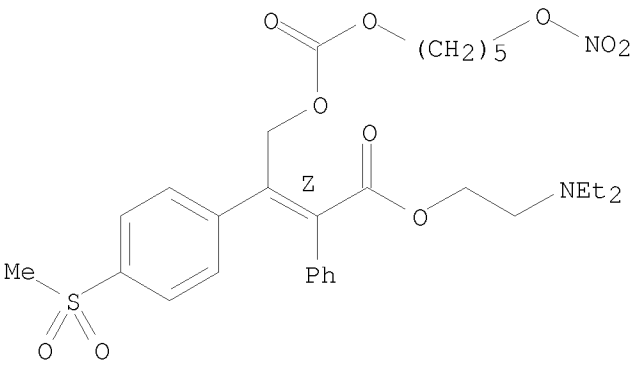
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethyl

ester, hydrochloride (1:1), (αZ)-
MF C29 H38 N2 O10 S . Cl H

Double bond geometry as shown.



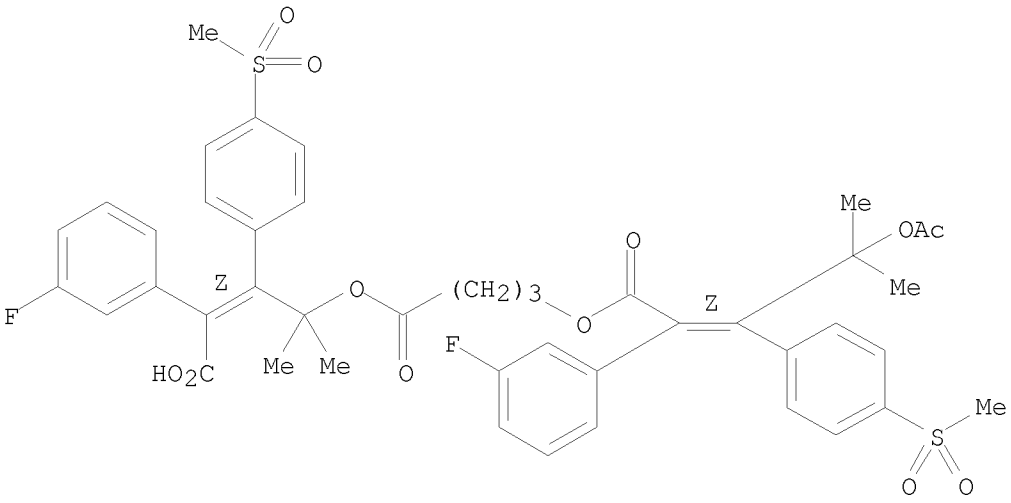
● HCl

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[4-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-1-oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, (αZ)-
MF C44 H44 F2 O12 S2
CI COM

Double bond geometry as shown.

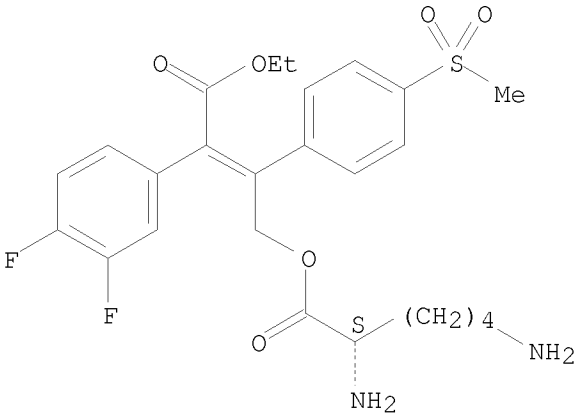


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester (9CI)
MF C25 H30 F2 N2 O6 S

Absolute stereochemistry.
Double bond geometry unknown.

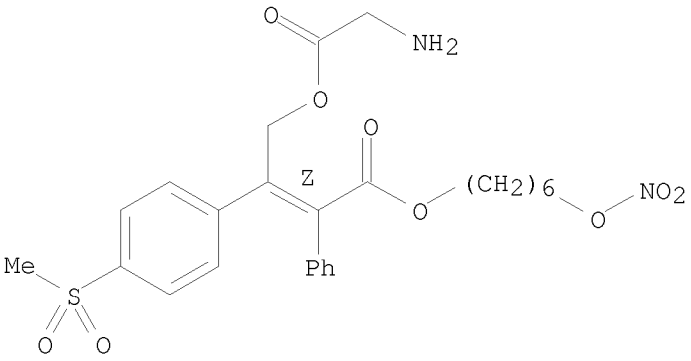


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester
MF C25 H30 N2 O9 S
CI COM

Double bond geometry as shown.

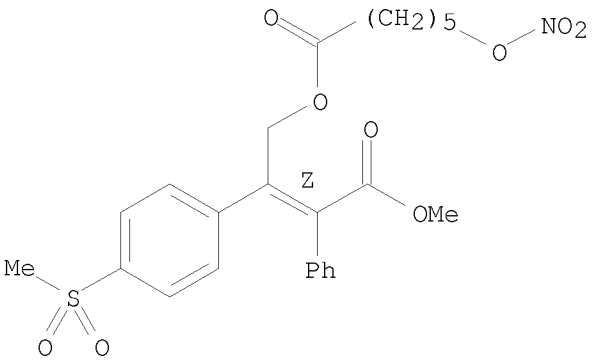


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, methyl ester, (αZ)-
MF C24 H27 N O9 S

Double bond geometry as shown.

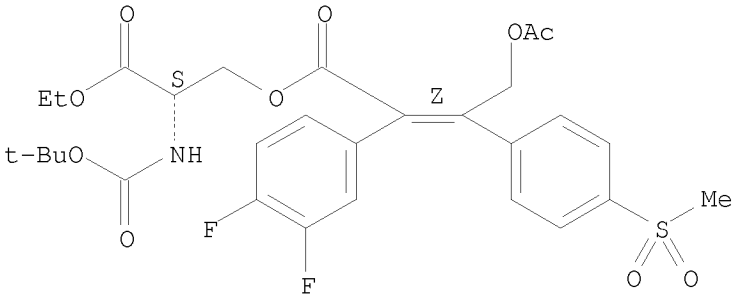


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-ethoxy-3-oxopropyl ester, (αZ)-
MF C29 H33 F2 N O10 S

Absolute stereochemistry.
Double bond geometry as shown.

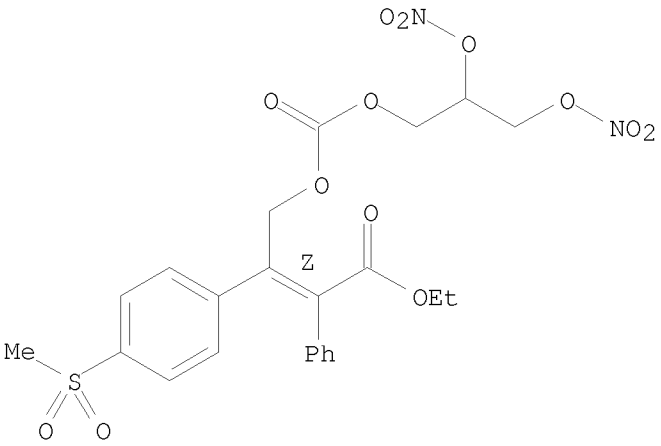


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)-
MF C23 H24 N2 O13 S

Double bond geometry as shown.

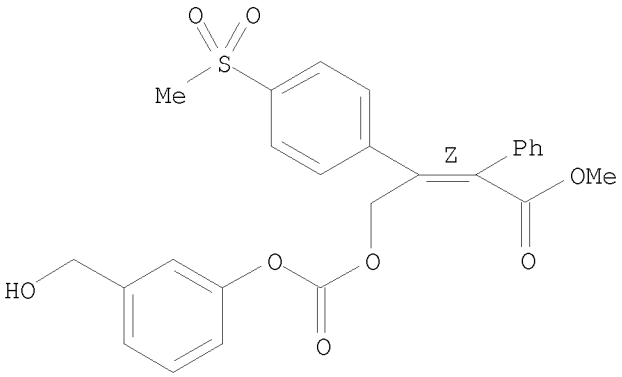


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[3-(hydroxymethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)-
MF C26 H24 O8 S

Double bond geometry as shown.

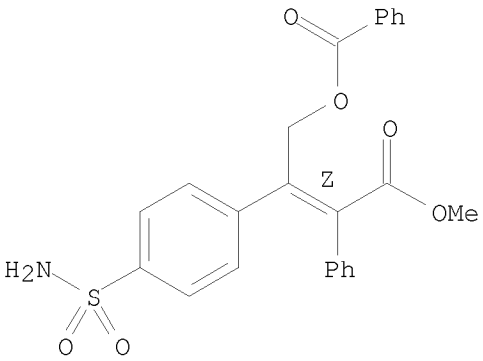


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(aminosulfonyl)phenyl]-2-(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI)
MF C24 H21 N O6 S

Double bond geometry as shown.

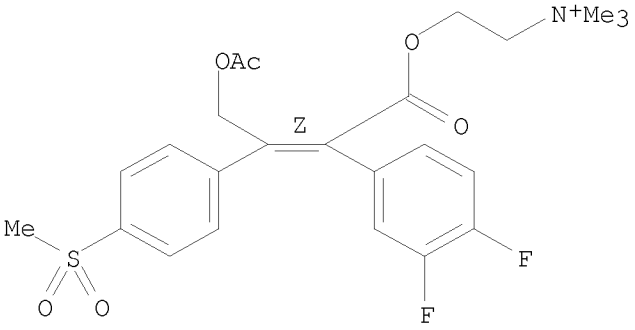


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

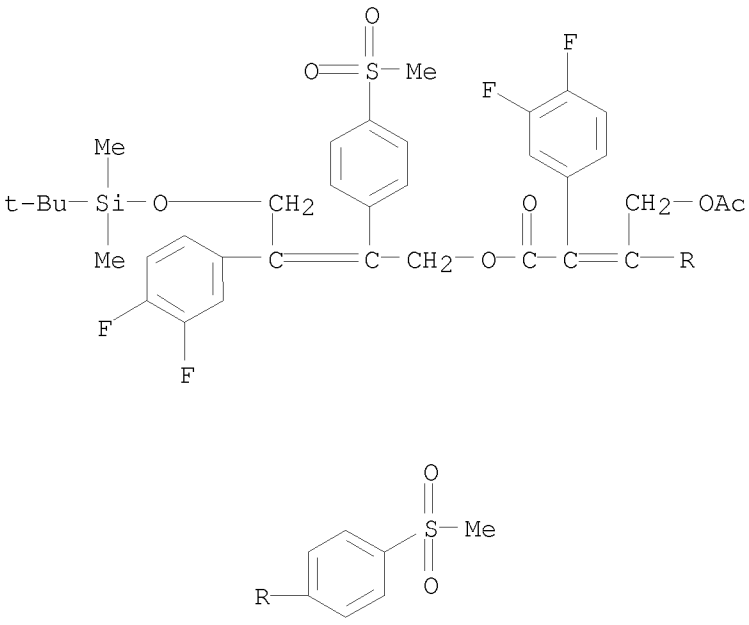
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-
MF C24 H28 F2 N O6 S
CI COM

Double bond geometry as shown.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, 3-(3,4-difluorophenyl)-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-[4-(methylsulfonyl)phenyl]-2-buten-1-yl ester
MF C42 H44 F4 O9 S2 Si

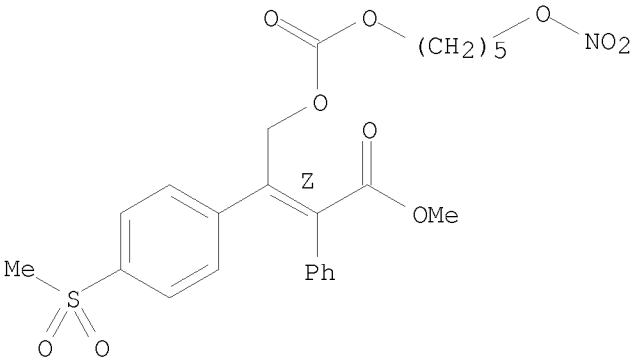


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (αZ)-
MF C24 H27 N O10 S

Double bond geometry as shown.

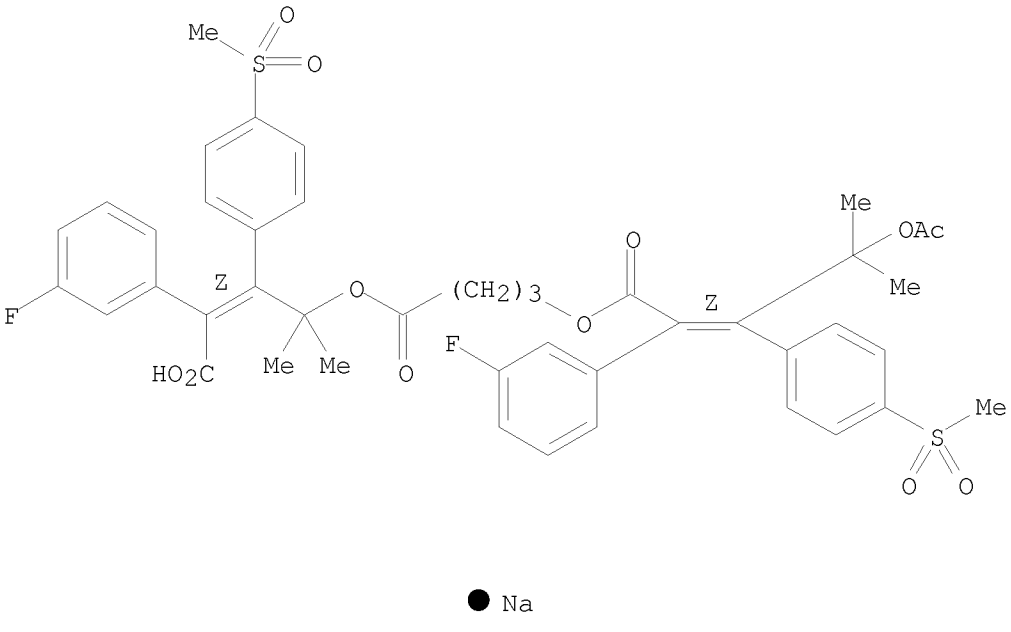


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C44 H44 F2 O12 S2 . Na

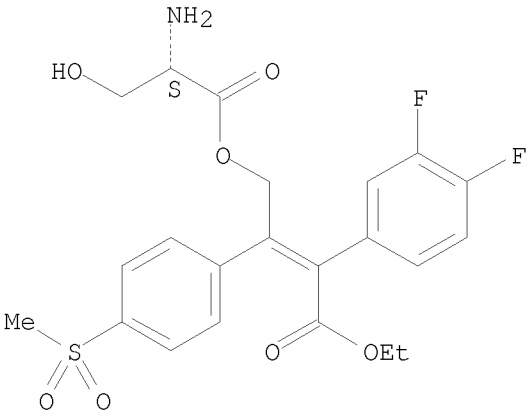
Double bond geometry as shown.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[(2S)-2-amino-3-hydroxy-1-oxopropoxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester (9CI)
MF C22 H23 F2 N O7 S

Absolute stereochemistry.
Double bond geometry unknown.

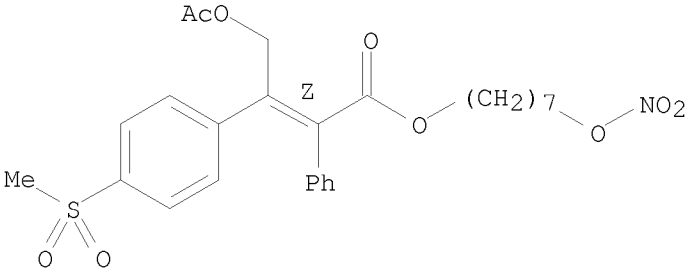


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 7-(nitrooxy)heptyl ester, (αZ)-
MF C26 H31 N O9 S

Double bond geometry as shown.



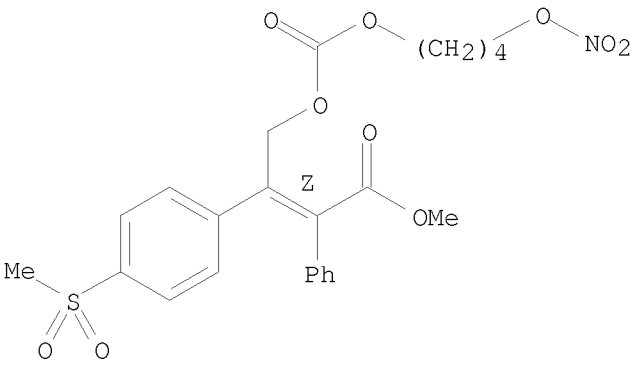
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, methyl ester, (αZ)-

MF C23 H25 N O10 S

Double bond geometry as shown.

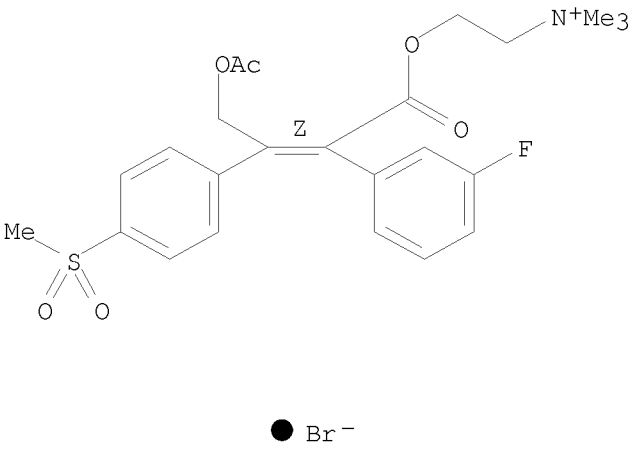


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
MF C24 H29 F N O6 S . Br

Double bond geometry as shown.

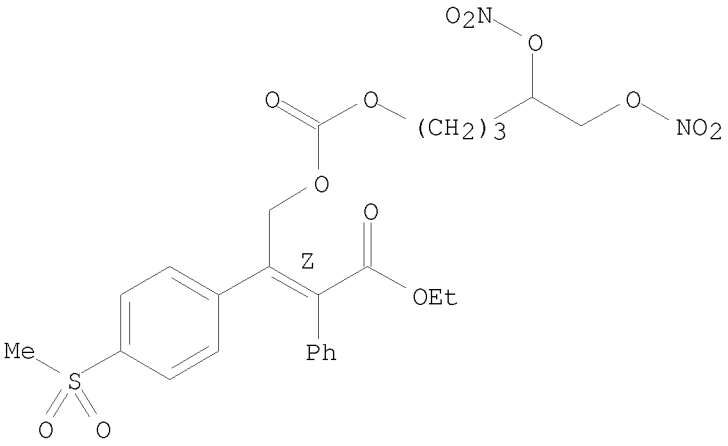


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[[4,5-

bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-
(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)-
MF C25 H28 N2 O13 S

Double bond geometry as shown.

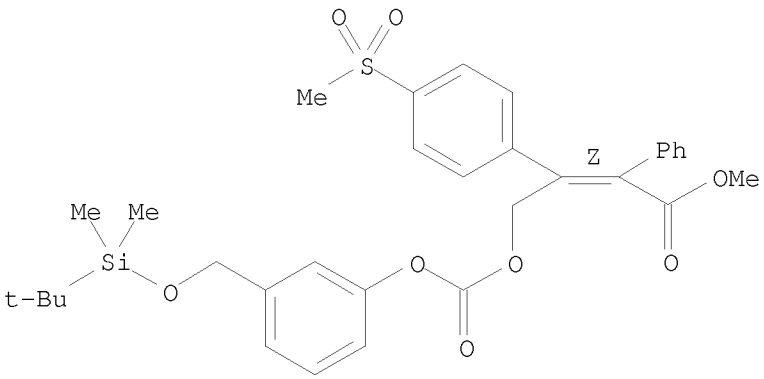


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[3-[[[(1,1-
dimethylethyl)dimethylsilyl]oxy]methyl]phenoxy]carbonyl]oxy]-1-[4-
(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)-
MF C32 H38 O8 S Si

Double bond geometry as shown.

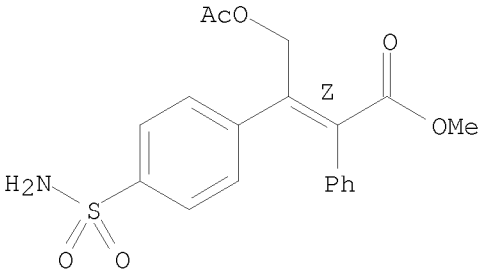


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI)
MF C19 H19 N O6 S

Double bond geometry as shown.

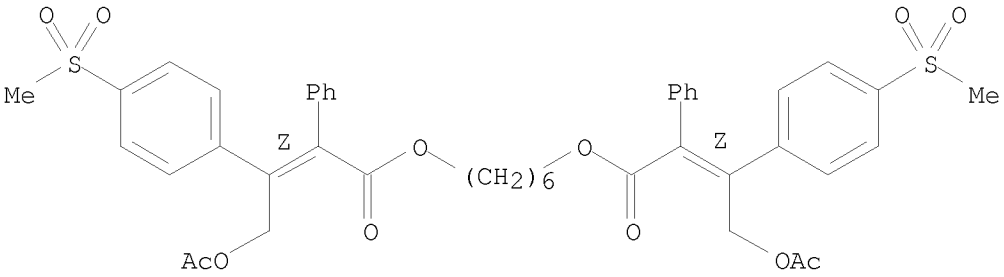


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

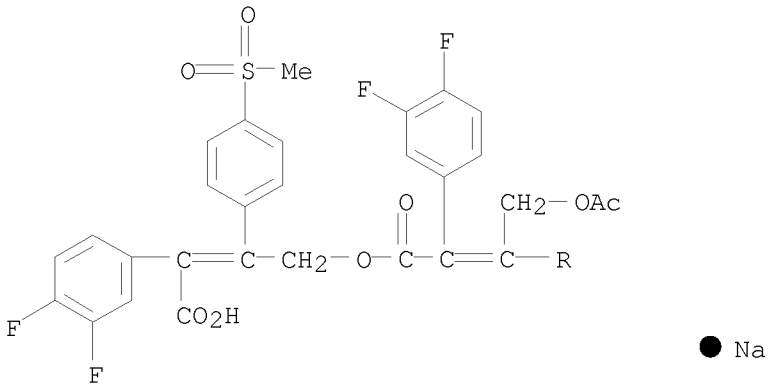
L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 1,6-hexanediyl ester, (αZ,α'Z)- (9CI)
MF C44 H46 O12 S2

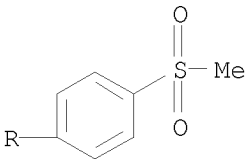
Double bond geometry as shown.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, sodium salt (1:1)
MF C36 H28 F4 O10 S2 . Na

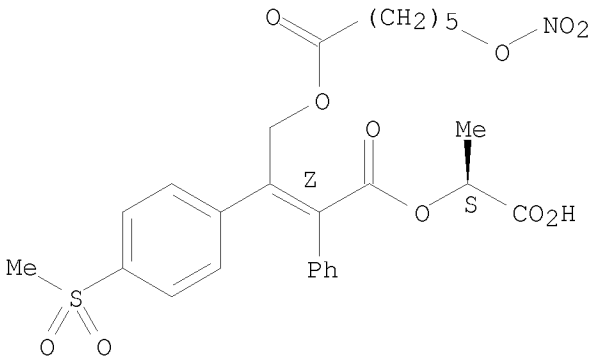




HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-1-carboxyethyl ester, (αZ)-
MF C26 H29 N O11 S

Absolute stereochemistry.
Double bond geometry as shown.

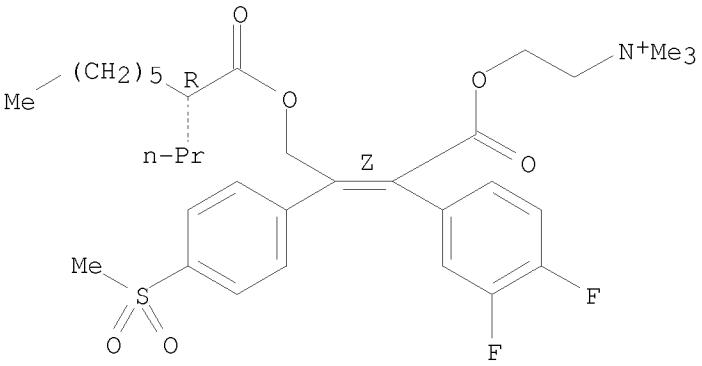


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-4-[[(2R)-1-oxo-2-propyloctyl]oxy]-2-buten-1-yl]oxy]-N,N,N-trimethyl-
MF C33 H46 F2 N O6 S
CI COM

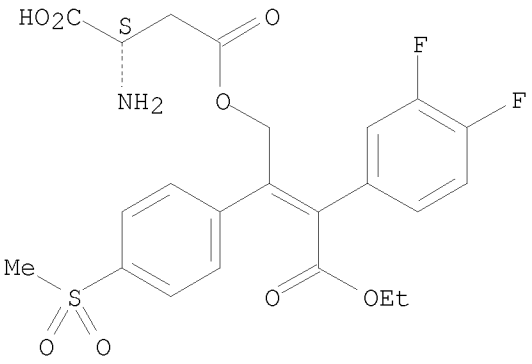
Absolute stereochemistry.
Double bond geometry as shown.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN L-Aspartic acid, 4-[3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester
MF C23 H23 F2 N O8 S

Absolute stereochemistry.
Double bond geometry unknown.



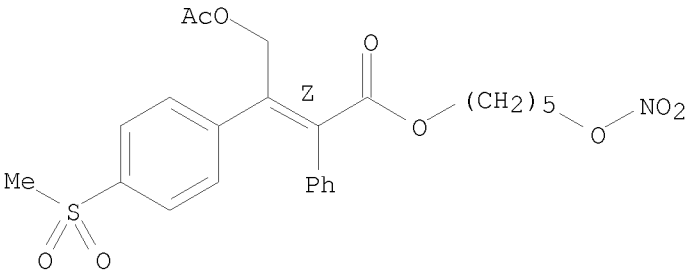
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 5-(nitrooxy)pentyl ester, (αZ)-
MF C24 H27 N O9 S

Double bond geometry as shown.

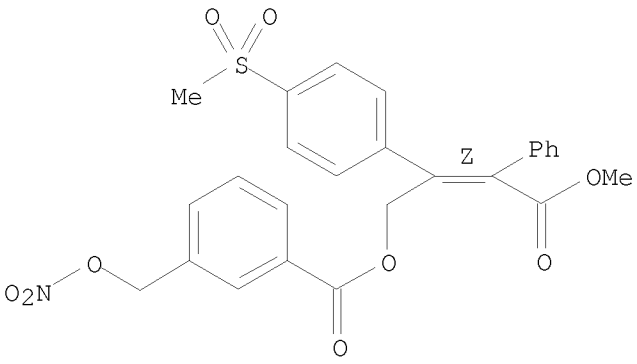


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[3-[(nitrooxy)methyl]benzoyl]oxy]ethylidene]-, methyl ester, (αZ)-
MF C26 H23 N O9 S

Double bond geometry as shown.

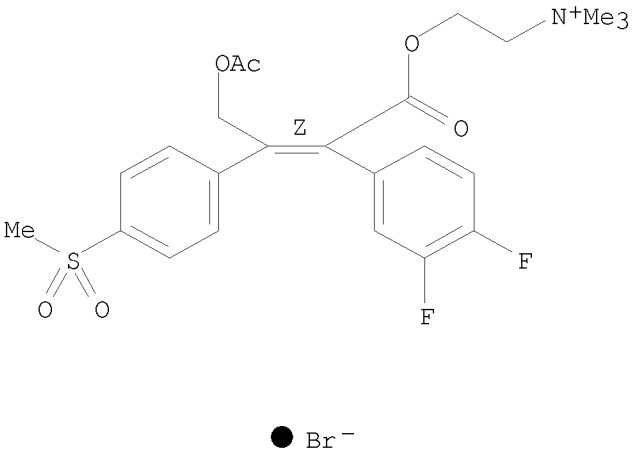


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
MF C24 H28 F2 N O6 S . Br

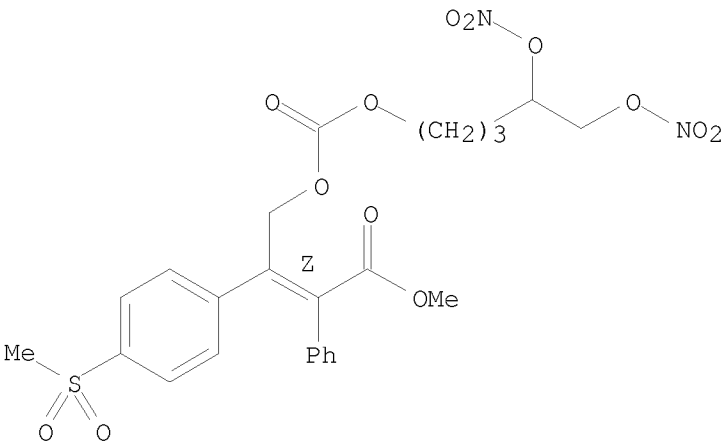
Double bond geometry as shown.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)-
MF C24 H26 N2 O13 S

Double bond geometry as shown.

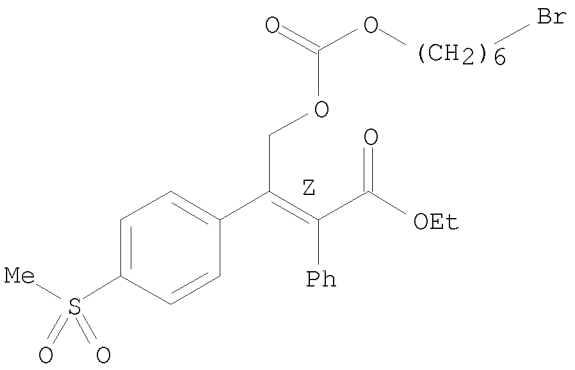


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)-
MF C26 H31 Br O7 S

Double bond geometry as shown.

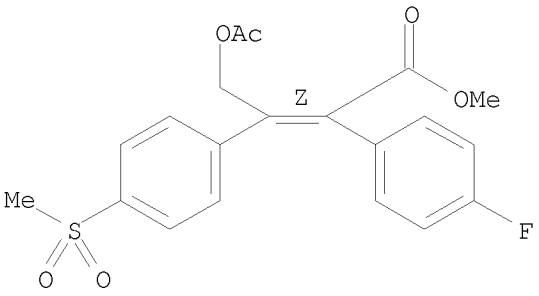


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI)
MF C20 H19 F O6 S

Double bond geometry as shown.

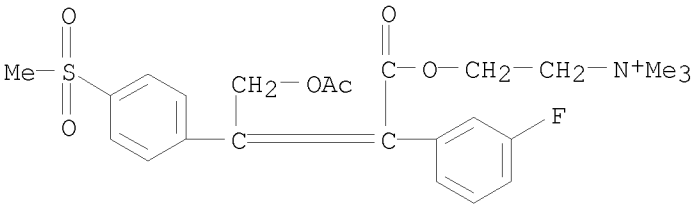


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-

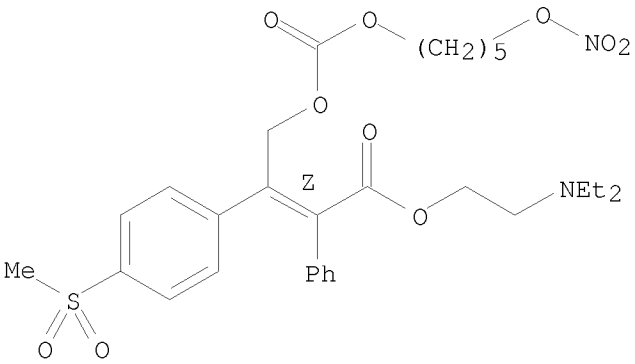
MF C24 H29 F N O6 S
CI COM



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, (αZ)-
MF C29 H38 N2 O10 S
CI COM

Double bond geometry as shown.

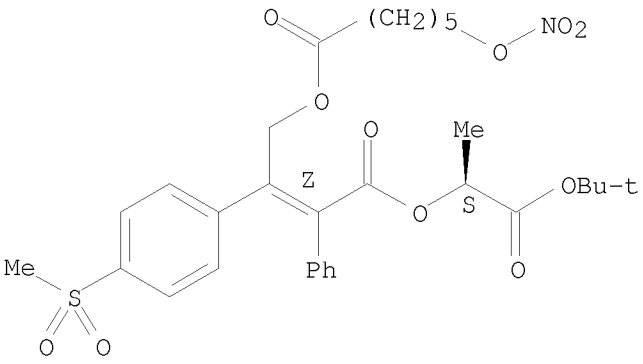


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl ester, (αZ)-
MF C30 H37 N O11 S

Absolute stereochemistry.
Double bond geometry as shown.

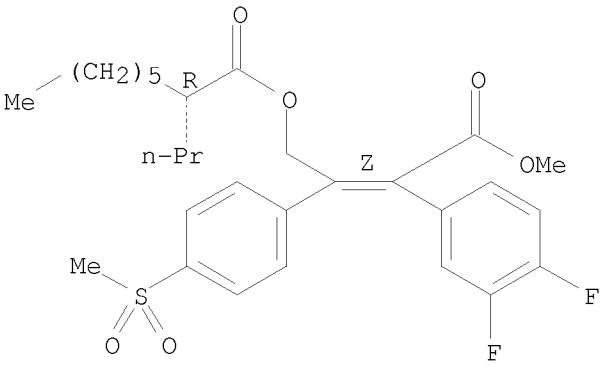


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, 3,4-difluoro-α-[1-[4-(methylsulfonyl)phenyl]-2-[[(2R)-1-oxo-2-propyloctyl]oxy]ethylidene]-, methyl ester, (αZ)-
MF C29 H36 F2 O6 S

Absolute stereochemistry.
Double bond geometry as shown.

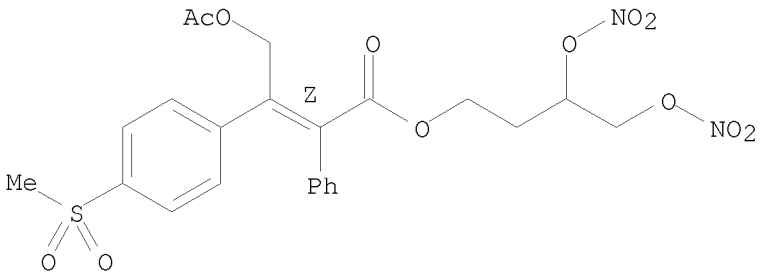


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, (αZ)-
MF C23 H24 N2 O12 S

Double bond geometry as shown.

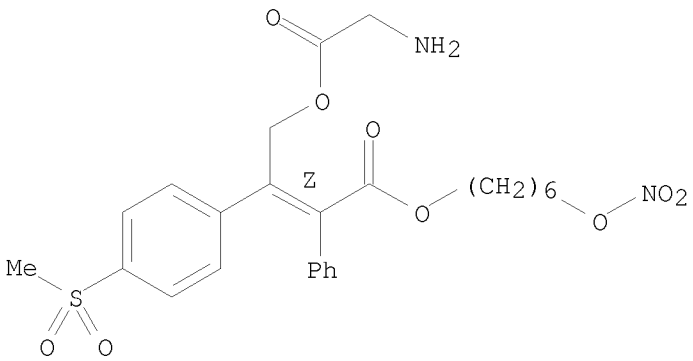


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-butenyl ester, monohydrochloride (9CI)
MF C25 H30 N2 O9 S . Cl H

Double bond geometry as shown.

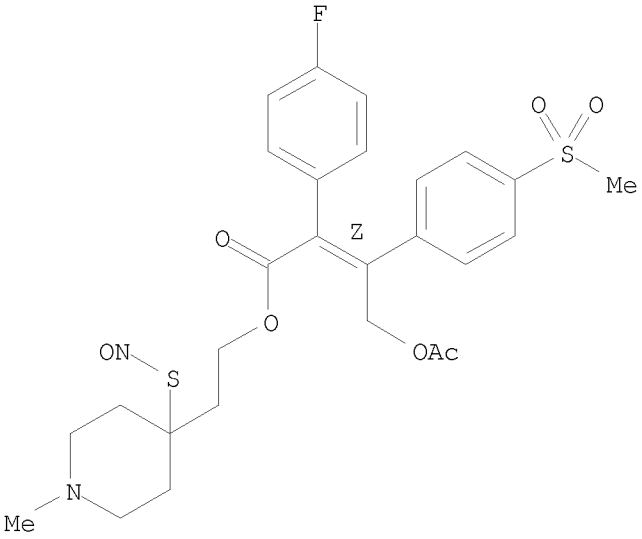


● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester, (αZ)-
MF C27 H31 F N2 O7 S2

Double bond geometry as shown.

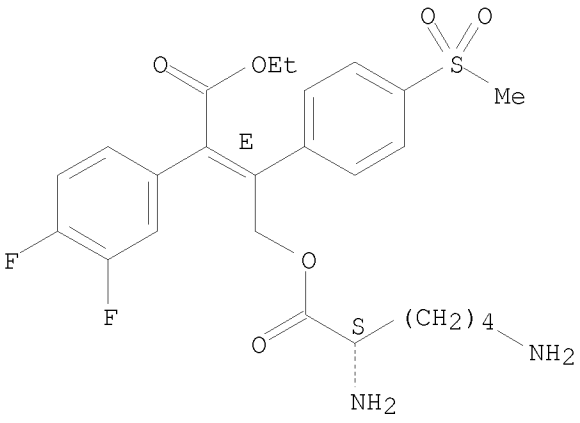


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester, (αE)- (9CI)
MF C25 H30 F2 N2 O6 S

Absolute stereochemistry.
Double bond geometry as shown.

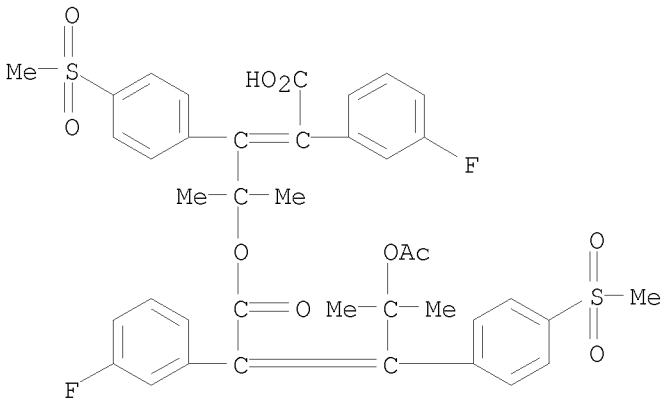


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-

3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-
MF C40 H38 F2 O10 S2
CI COM

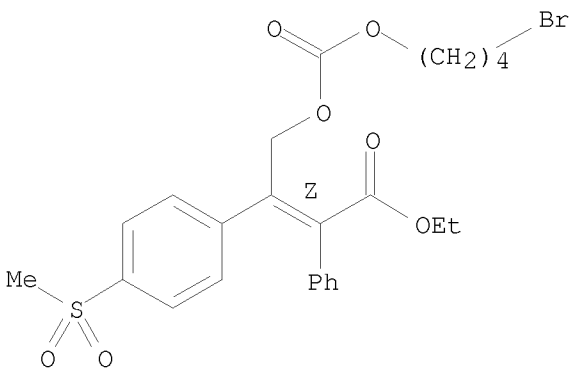


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)-
MF C24 H27 Br O7 S

Double bond geometry as shown.

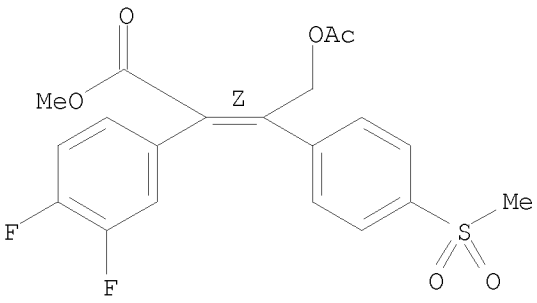


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI)
MF C20 H18 F2 O6 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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=> file zcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	201.24	201.46

FILE 'ZCAPLUS' ENTERED AT 11:14:23 ON 17 JUN 2009
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FILE COVERS 1907 - 17 Jun 2009 VOL 150 ISS 25
FILE LAST UPDATED: 15 Jun 2009 (20090615/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> e us2006-586573/apps

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E2	2	US2006-586567/AP

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E4            0     US2006-586573/PRN
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E6            1     US2006-586575/AP
E7            1     US2006-586576/AP
E8            1     US2006-586577/AP
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E10           1     US2006-586579/AP
E11           1     US2006-586581/AP
E12           1     US2006-586583/AP

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              0 US2006-586573/PRN
L4            1 US2006-586573/APPS
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=> sel rn
E1 THROUGH E34 ASSIGNED

=> file registry
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FULL ESTIMATED COST                                       5.90     207.36

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STRUCTURE FILE UPDATES:   15 JUN 2009  HIGHEST RN 1158168-92-3
DICTIONARY FILE UPDATES:  15 JUN 2009  HIGHEST RN 1158168-92-3

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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                  (108-24-7/RN)
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I OR 654068-92-5/BI OR 6835-50-3/BI OR 754242-03-0/BI OR 77-76-9
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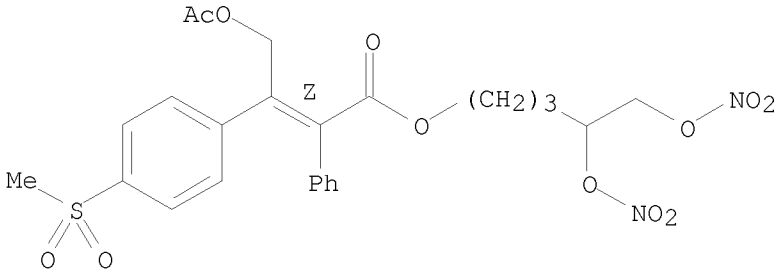
861655-83-6/BI OR 861655-84-7/BI OR 861655-85-8/BI OR 861655-86-
9/BI)

=> s l3 and l5
L6 4 L3 AND L5

=> d sca

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester,
(αZ)-
MF C24 H26 N2 O12 S

Double bond geometry as shown.

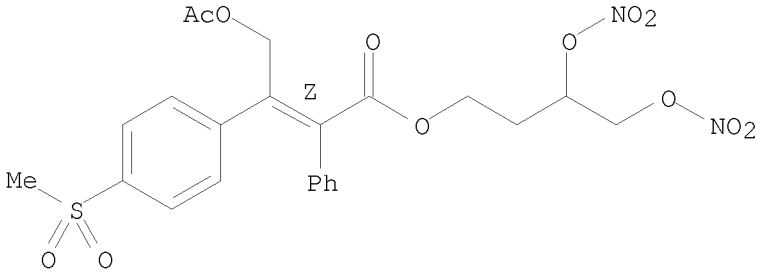


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester,
(αZ)-
MF C23 H24 N2 O12 S

Double bond geometry as shown.

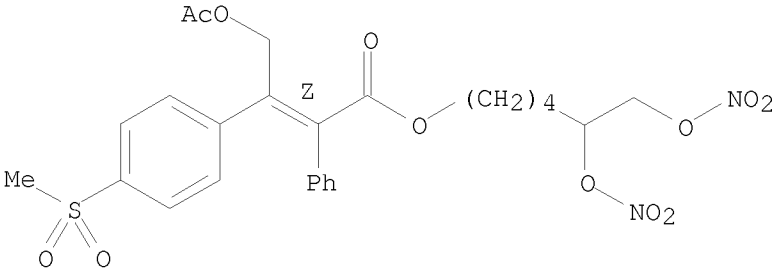


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)-
MF C25 H28 N2 O12 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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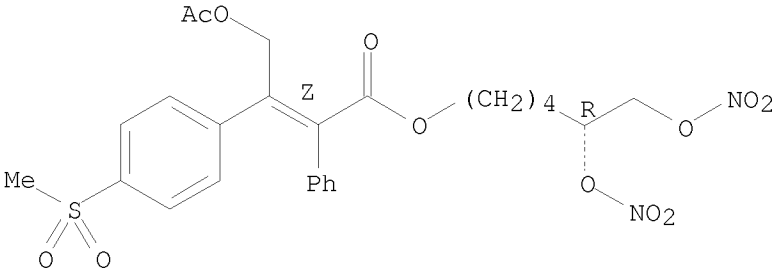
L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (αZ)-
MF C25 H28 N2 O12 S

Absolute stereochemistry.
Double bond geometry as shown.



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```
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SESSION CONTINUES IN FILE 'REGISTRY'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available.  If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       2.40     209.76

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FILE COVERS 1907 - 17 Jun 2009  VOL 150 ISS 25
FILE LAST UPDATED: 15 Jun 2009  (20090615/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Feb 2009

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3
L7          18 L3

=> s l7 and (nitrosated or nitrosylated)
          1340 NITROSATED
           604 NITROSYLATED
L8           1 L7 AND (NITROSATED OR NITROSYLATED)

=> d sca

L8    1 ANSWERS   ZCAPLUS  COPYRIGHT 2009 ACS on STN
IC   ICM  A61K031-40
     ICS  A61K031-415; A61K031-421; A61K031-50; C07D207-325; C07D231-06;
          C07D237-14; C07D263-04; C07D263-06
CC   21-2 (General Organic Chemistry)
     Section cross-reference(s): 1
TI   Preparation of nitrosated and nitrosylated
```

cyclooxygenase-2 inhibitors

ST cyclooxygenase 2 inhibitor nitrosated nitrosylated prepn

IT Analgesics
Anti-inflammatory agents
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

IT Nitroso compounds
Nitrosyl complexes
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

IT 329900-75-6, cyclooxygenase-2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(mediated disorders; treatment; preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

IT 205580-05-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

IT 346683-69-0P 346683-70-3P 346683-71-4P 346683-72-5P 346683-73-6P
346683-75-8P 346683-76-9P 346683-77-0P 346683-78-1P 346683-79-2P
346683-80-5P 346683-81-6P 346683-82-7P 346683-83-8P
346683-84-9P 346683-85-0P 346683-86-1P 346683-87-2P 346683-88-3P
347162-90-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

IT 346683-99-6P 346684-20-6P 346684-22-8P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

IT 52-67-5, D-Penicillamine 53-86-1, Indomethacin 78-83-1, 2-Methyl-1-propanol, reactions 78-94-4, Methyl vinyl ketone, reactions 100-53-8, Benzyl mercaptan 627-18-9, 3-Bromo-1-propanol 1445-73-4, 1-Methyl-4-piperidone 1778-09-2, 4-Methylthioacetophenone 2417-72-3, Methyl 4-bromomethylbenzoate 3446-89-7, 4-Methylthiobenzaldehyde 18162-48-6, tert-Butyldimethylsilyl chloride 21382-98-9, 4-Methylthiobenzonitrile 24214-73-1, Cyclohexylhydrazine hydrochloride 32047-53-3, 1-Amino-2-methyl-2-propanethiol hydrochloride 61040-78-6, 2,4,6-Trimethoxybenzyl alcohol 90878-19-6, Phenethylmagnesium chloride 194596-99-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

IT 15581-80-3P 28399-82-8P 40027-88-1P 73303-88-5P, 2-Methyl-2-mercapto-1-propanol 86864-60-0P 89031-84-5P 136881-95-3P
157672-00-9P 170571-19-4P 170571-20-7P 170571-71-8P 179174-91-5P
179174-92-6P 179174-93-7P 179174-94-8P 181695-72-7P 181695-81-8P
189501-33-5P 189501-34-6P 205579-90-4P 213763-90-7P 213764-17-1P
215124-07-5P 215124-20-2P 291518-72-4P 346683-89-4P 346683-90-7P
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346683-97-4P 346683-98-5P 346684-00-2P 346684-01-3P 346684-02-4P
346684-03-5P 346684-04-6P 346684-05-7P 346684-06-8P 346684-07-9P

346684-08-0P 346684-09-1P 346684-10-4P 346684-11-5P 346684-12-6P
346684-13-7P 346684-14-8P 346684-15-9P 346684-16-0P 346684-17-1P
346684-18-2P 346684-19-3P 346684-21-7P 347162-91-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)
IT 346684-23-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

ALL ANSWERS HAVE BEEN SCANNED

=> s l7 and (nitrosated or nitrosylated or NO or (nitric (w) oxide))
1340 NITROSATED
604 NITROSYLATED
3932570 NO
220094 NOS
2032 NOES
4060112 NO
(NO OR NOS OR NOES)
223122 NITRIC
3 NITRICS
223125 NITRIC
(NITRIC OR NITRICS)
1991269 OXIDE
377613 OXIDES
2097881 OXIDE
(OXIDE OR OXIDES)
131578 NITRIC (W) OXIDE
L9 11 L7 AND (NITROSATED OR NITROSYLATED OR NO OR (NITRIC (W) OXIDE))

=> d sca

L9 11 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN
IC ICM C07C317-24
ICS A61K031-21
INCL 514509000; 558482000
CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1
TI Process for making nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors
ST nitric oxide releasing prodrug diphenylbutenoate hexyl nitrate
IT Drug delivery systems
(prodrugs; preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT 329900-75-6, Cyclooxygenase 2
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT 10102-43-9, Nitric oxide, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT 64-19-7, Acetic acid, uses 67-68-5, Dmso, uses 68-12-2, Dmf, uses 75-05-8, Acetonitrile, uses 75-09-2, Dichloromethane, uses 75-52-5, Nitromethane, uses 127-19-5, N,N-Dimethylacetamide 872-50-4, 1-Methyl-2-pyrrolidinone, uses 1300-21-6, Dichloroethane 25321-22-6, Dichlorobenzene

RL: NUU (Other use, unclassified); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

IT 937-14-4, m-Chloroperbenzoic acid 1504-58-1, 3-Phenyl-2-propyn-1-ol 4286-55-9 7722-84-1, Hydrogen peroxide, reactions 10058-23-8, Potassium peroxymonosulfate 11138-47-9, Sodium perborate 74087-85-7, Dimethyldioxirane 78948-87-5, Magnesium monoperoxyphthalate 210292-04-9, 4-Methylthiophenylmagnesium chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

IT 176594-44-8P 179174-79-9P 754242-10-9P 754242-11-0P 754242-12-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

IT 754241-98-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

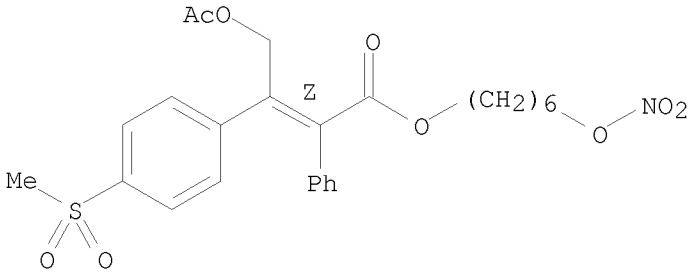
=> d ibib hitstr 1-11
THE ESTIMATED COST FOR THIS REQUEST IS 42.79 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L9 ANSWER 1 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:465556 ZCAPLUS
DOCUMENT NUMBER: 148:523285
TITLE: Development of a discriminating in vitro dissolution method for a poorly soluble NO-donating selective cyclooxygenase-2 inhibitor
AUTHOR(S): Papp, Robert; Luk, Pauline; Mullett, Wayne M.; Kwong, Elizabeth; Debnath, Smita; Thibert, Roch
CORPORATE SOURCE: Drug Metabolism and Pharmacokinetics, Merck Frosst Center for Therapeutic Research, Kirkland, QC, H9H 3L1, Can.
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (2008), 47(1), 16-22
CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

IT 754241-98-0
RL: PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(development of discriminating in vitro dissoln. method for poorly soluble NO-donating cyclooxygenase-2 inhibitor)

RN 754241-98-0 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:495882 ZCAPLUS
DOCUMENT NUMBER: 145:14695
TITLE: Compounds for targeting mechanisms implicated in the progression of stroke
INVENTOR(S): Munoz, Benito; Payne, Joseph E.; Prasit, Petpiboon; Reger, Thomas S.; Smith, Nicholas D.; Stock, Nicholas S.; McGuire, Angela R.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

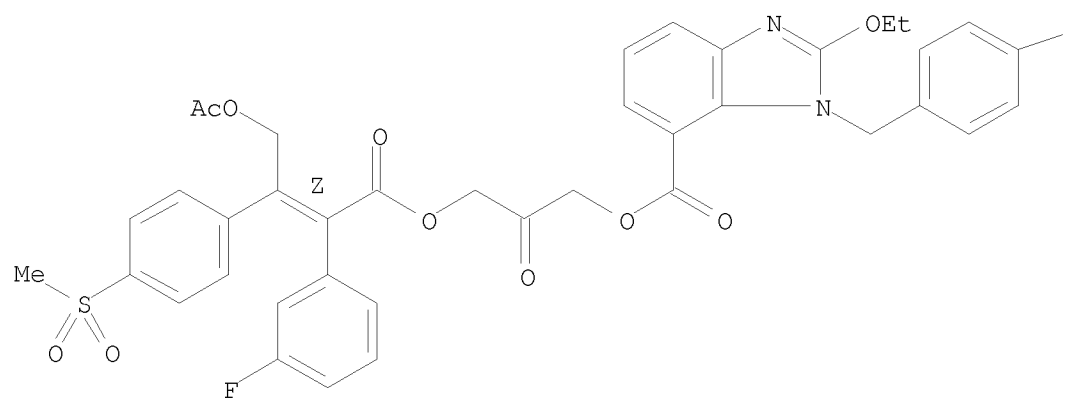
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006055404	A2	20060526	WO 2005-US40851	20051110
WO 2006055404	A3	20060810		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

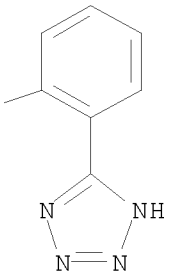
PRIORITY APPLN. INFO.: US 2004-628280P P 20041116
OTHER SOURCE(S): MARPAT 145:14695
IT 887908-51-2P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(compds. for targeting mechanisms implicated in progression of stroke)
RN 887908-51-2 ZCAPLUS
CN 1H-Benzimidazole-7-carboxylic acid, 2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, 3-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-2-oxopropyl ester (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

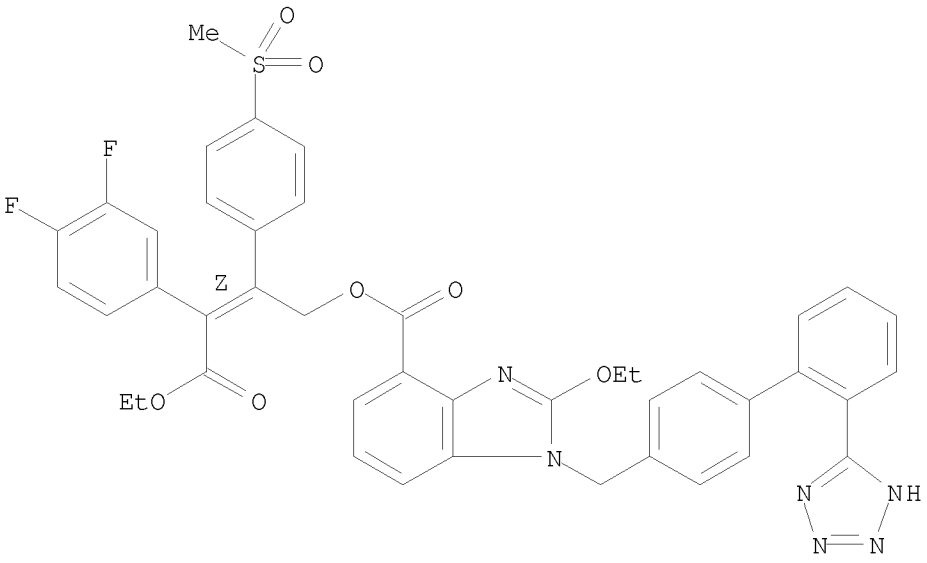


PAGE 1-B



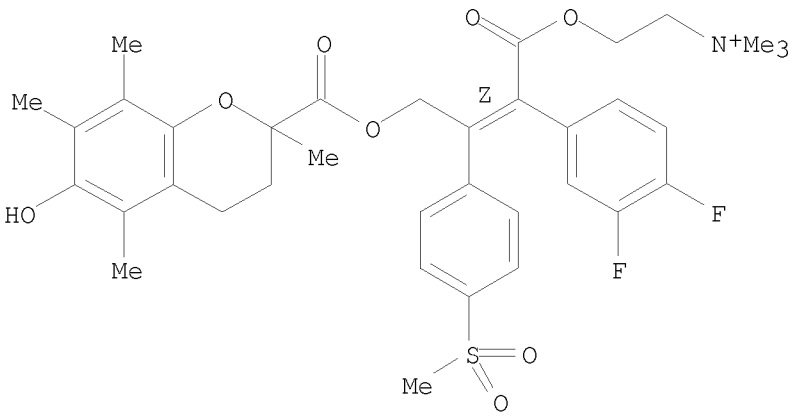
IT 887908-54-5 887908-56-7
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compds. for targeting mechanisms implicated in progression of stroke)
RN 887908-54-5 ZCAPLUS
CN 1H-Benzimidazole-4-carboxylic acid, 2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, (2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 887908-56-7 ZCAPLUS
CN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-4-[[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)carbonyl]oxy]-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:383478 ZCAPLUS
DOCUMENT NUMBER: 144:432558
TITLE: Preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors.
INVENTOR(S): Munoz, Benito; Payne, Joseph Edward; Prasit, Petpiboon; Reger, Thomas S.; Smith, Nicholas D.; Stock, Nicholas S.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

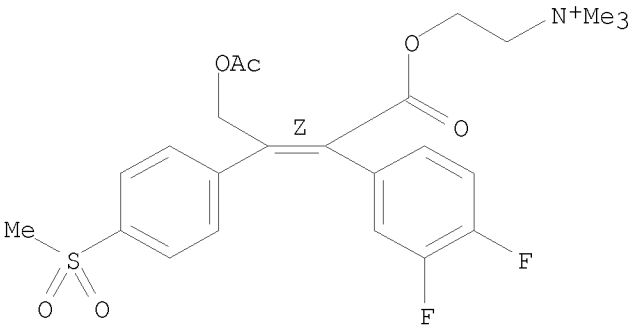
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006044230	A1	20060427	WO 2005-US36031	20051007

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

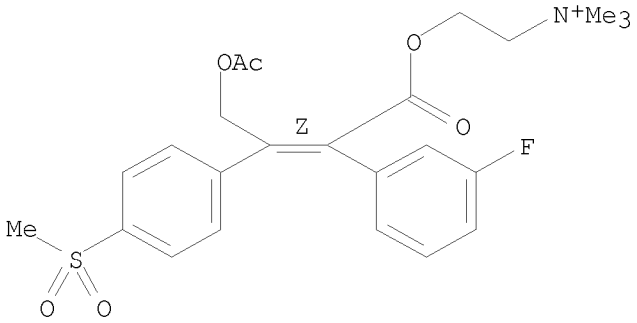
PRIORITY APPLN. INFO.: US 2004-617962P P 20041012
OTHER SOURCE(S): MARPAT 144:432558
IT 885020-33-7P 885020-34-8P 885020-36-0P
885020-37-1P 885020-38-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of methylsulfonylphenylalkenoates as water soluble
prodrugs of COX-2 inhibitors)
RN 885020-33-7 ZCAPLUS
CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl- (CA INDEX NAME)

Double bond geometry as shown.



RN 885020-34-8 ZCAPLUS
CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl- (CA INDEX NAME)

Double bond geometry as shown.

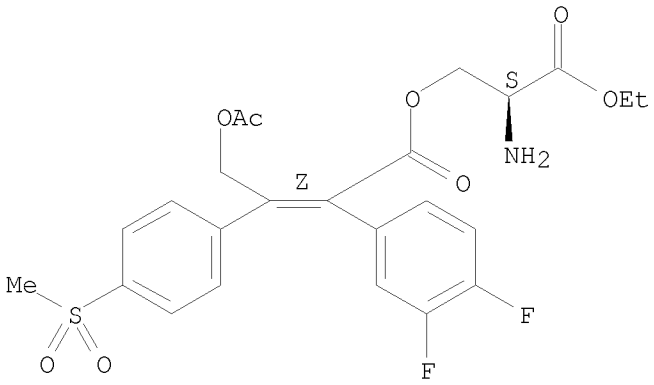


RN 885020-36-0 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (αZ)-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

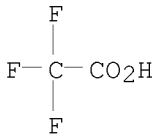
CRN 885020-35-9
CMF C24 H25 F2 N O8 S

Absolute stereochemistry.
Double bond geometry as shown.



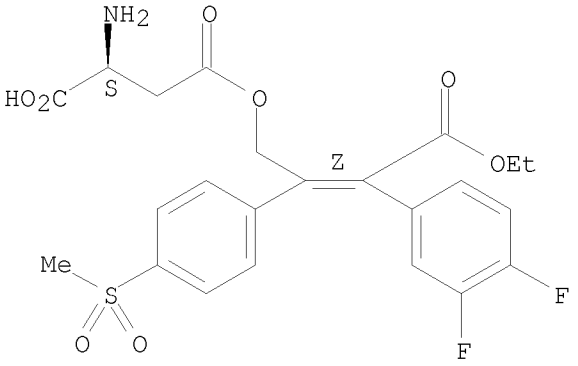
CM 2

CRN 76-05-1
CMF C2 H F3 O2



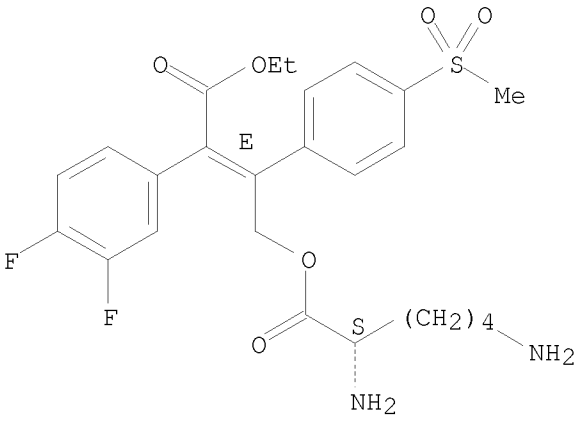
RN 885020-37-1 ZCAPLUS
CN L-Aspartic acid, 4-[(2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



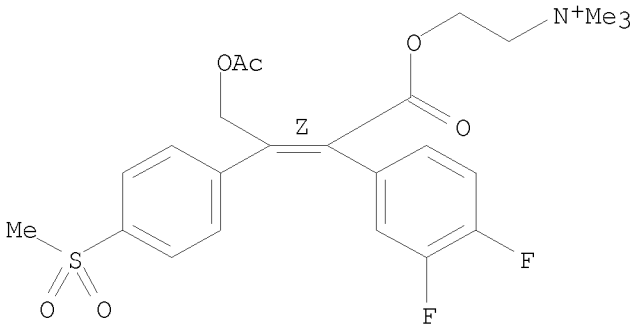
RN 885020-38-2 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester, (αE)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 885020-42-8P 885020-43-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors)
RN 885020-42-8 ZCAPLUS
CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1) (CA INDEX NAME)

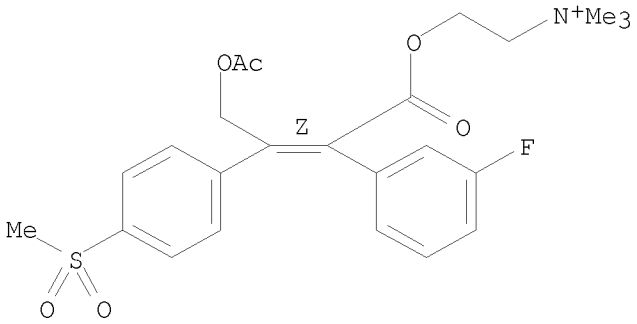
Double bond geometry as shown.



● Br^-

RN 885020-43-9 ZCAPLUS
CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1) (CA INDEX NAME)

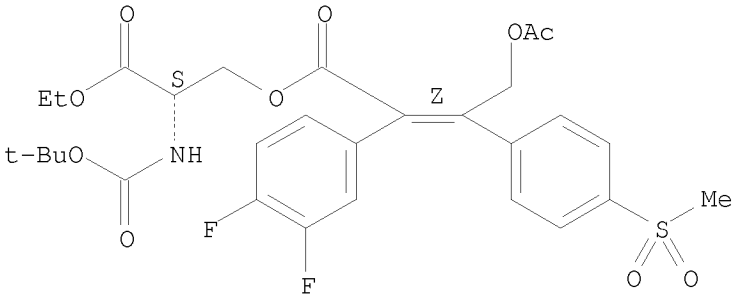
Double bond geometry as shown.



● Br^-

IT 885020-47-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors)
RN 885020-47-3 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-ethoxy-3-oxopropyl ester, (αZ)- (CA INDEX NAME)

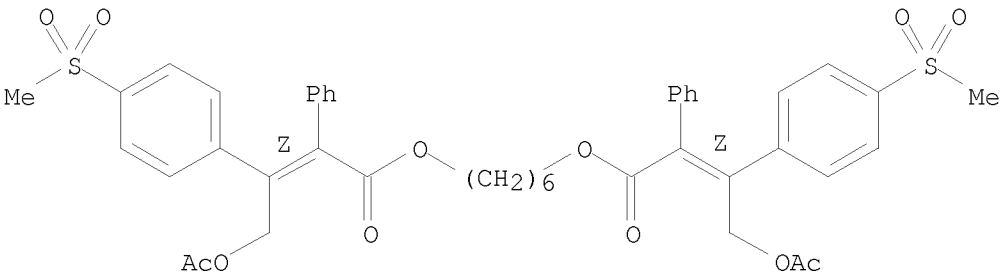
Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1315893 ZCAPLUS
DOCUMENT NUMBER: 144:212486
TITLE: Synthesis of a NO-Releasing Prodrug of Rofecoxib
AUTHOR(S): Engelhardt, F. Conrad; Shi, Yao-Jun; Cowden, Cameron J.; Conlon, David A.; Pipik, Brenda; Zhou, George; McNamara, James M.; Dolling, Ulf-H.
CORPORATE SOURCE: Department of Process Research, Merck Company, Rahway, NJ, 07065-0900, USA
SOURCE: Journal of Organic Chemistry (2006), 71(2), 480-491
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:212486
IT 875783-67-8P
RL: BYP (Byproduct); PREP (Preparation)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
RN 875783-67-8 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 1,6-hexanediyl ester, (αZ,α'Z)- (9CI) (CA INDEX NAME)

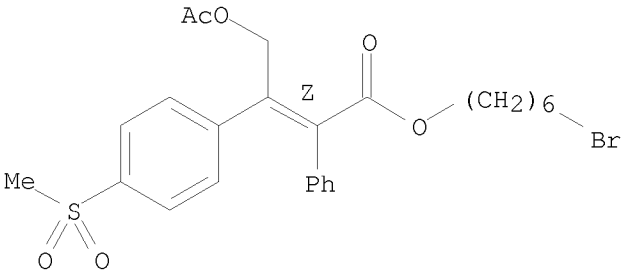
Double bond geometry as shown.



IT 754242-04-1P
RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
RN 754242-04-1 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-

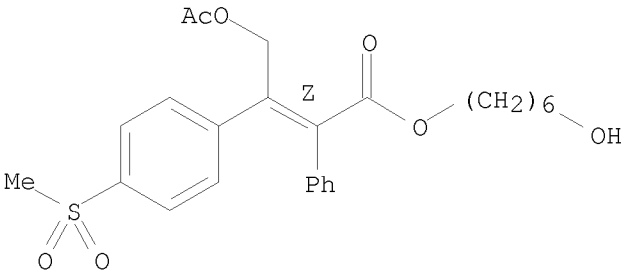
(methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



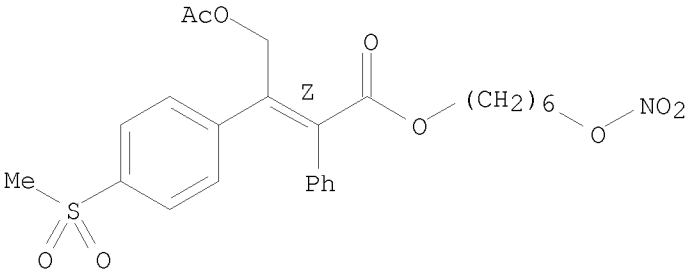
IT 754242-12-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
RN 754242-12-1 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



IT 754241-98-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
RN 754241-98-0 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



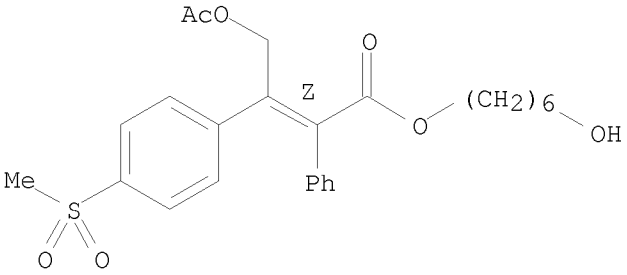
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:963804 ZCAPLUS
DOCUMENT NUMBER: 143:266677
TITLE: Process for making nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors
INVENTOR(S): Shi, Yao-Jun; Engelhardt, F. Conrad; Cowden, Cameron John; Conlon, David A.; Pipik, Brenda
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 16 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20050192346	A1	20050901	US 2005-66676		20050225
PRIORITY APPLN. INFO.:			US 2004-549126P	P	20040301

OTHER SOURCE(S): CASREACT 143:266677; MARPAT 143:266677
IT 754242-12-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
RN 754242-12-1 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (αZ)-(CA INDEX NAME)

Double bond geometry as shown.



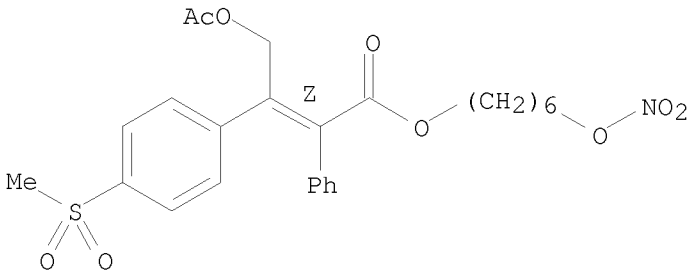
IT 754241-98-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 754241-98-0 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



L9 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:696873 ZCAPLUS

DOCUMENT NUMBER: 143:172624

TITLE: Preparation of nitric oxide releasing prodrugs of diaryl-2(5H)-furanones as cyclooxygenase-2 inhibitors

INVENTOR(S): Dufresne, Claude; Berthelette, Carl; Li, Lianhai; Guay, Daniel; Gallant, Michel; Lacombe, Patrick; Aspiotis, Renee; Wang, Zhaoyin; Sturino, Claudio F.

PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.

SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

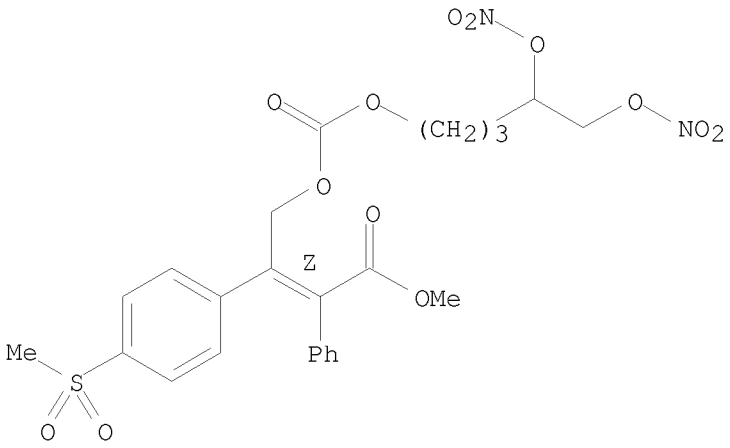
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070883	A1	20050804	WO 2005-CA83	20050125
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005206228	A1	20050804	AU 2005-206228	20050125
CA 2554334	A1	20050804	CA 2005-2554334	20050125
EP 1711459	A1	20061018	EP 2005-706413	20050125
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1914169	A	20070214	CN 2005-80003263	20050125
JP 2007520483	T	20070726	JP 2006-549814	20050125

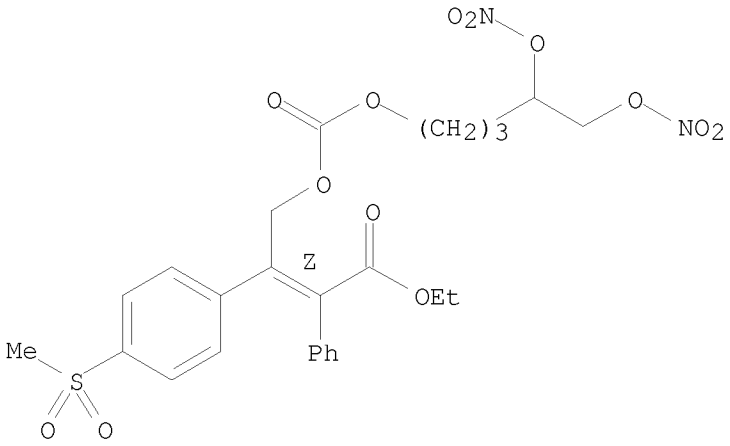
US 20080242643 A1 20081002 US 2006-586381 20060718
IN 2006DN04347 A 20070713 IN 2006-DN4347 20060727
PRIORITY APPLN. INFO.: US 2004-539666P P 20040127
WO 2005-CA83 W 20050125
OTHER SOURCE(S): CASREACT 143:172624; MARPAT 143:172624
IT 861430-33-3P 861430-34-4P 861430-36-6P
861430-38-8P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diaryl-2(5H)-furanones as cyclooxygenase-2 inhibitors)
RN 861430-33-3 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



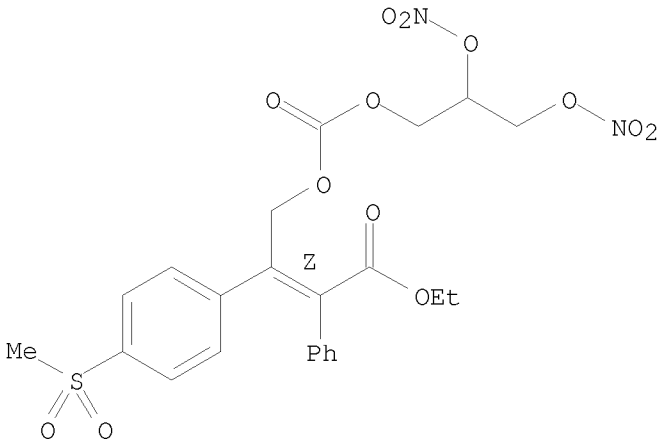
RN 861430-34-4 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



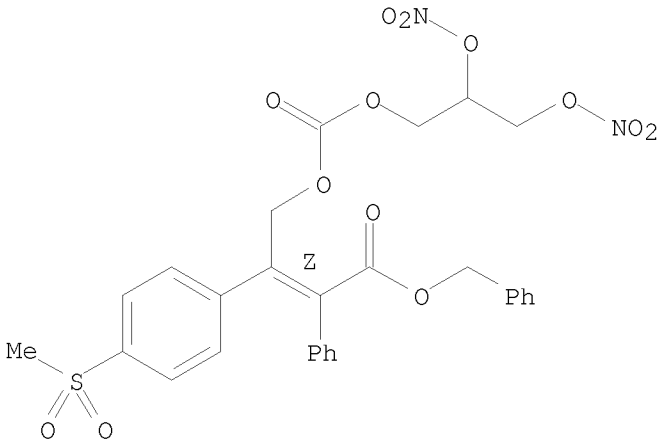
RN 861430-36-6 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 861430-38-8 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, phenylmethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:696865 ZCAPLUS
DOCUMENT NUMBER: 143:193802
TITLE: Preparation of nitric oxide releasing prodrugs of diaryl-2(5H)-furanones as cyclooxygenase-2 inhibitors
INVENTOR(S): Berthelette, Carl; Li, Lianhai; Beaulieu, Christian; Wang, Zhaoyin; Sturino, Claudio F.
PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070874	A1	20050804	WO 2005-CA84	20050125
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005206229	A1	20050804	AU 2005-206229	20050125
CA 2554333	A1	20050804	CA 2005-2554333	20050125
EP 1711457	A1	20061018	EP 2005-706414	20050125
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1914151	A	20070214	CN 2005-80003240	20050125
JP 2007520484	T	20070726	JP 2006-549815	20050125
US 20080227758	A1	20080918	US 2006-586573	20060718
IN 2006DN04343	A	20070713	IN 2006-DN4343	20060727
PRIORITY APPLN. INFO.:			US 2004-540101P P	20040127

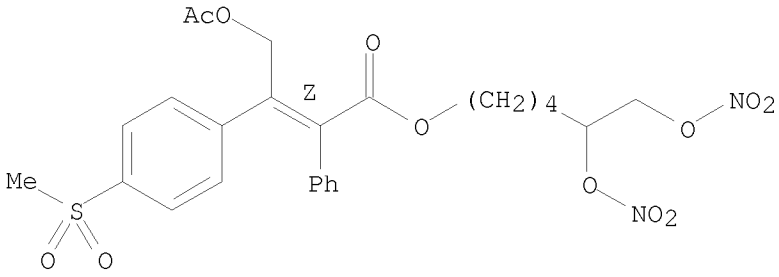
OTHER SOURCE(S): CASREACT 143:193802; MARPAT 143:193802

IT 861655-83-6P 861655-84-7P 861655-85-8P
861655-86-9P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diaryl-2(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 861655-83-6 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)- (CA INDEX NAME)

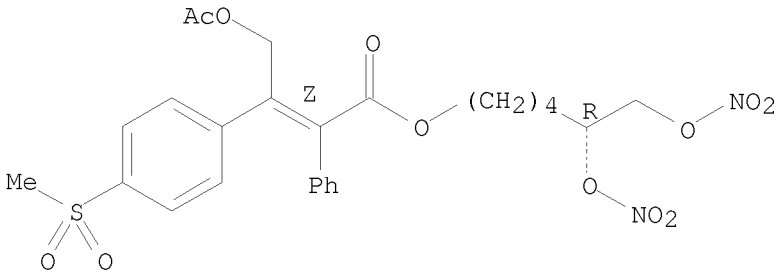
Double bond geometry as shown.



RN 861655-84-7 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (αZ)- (CA INDEX NAME)

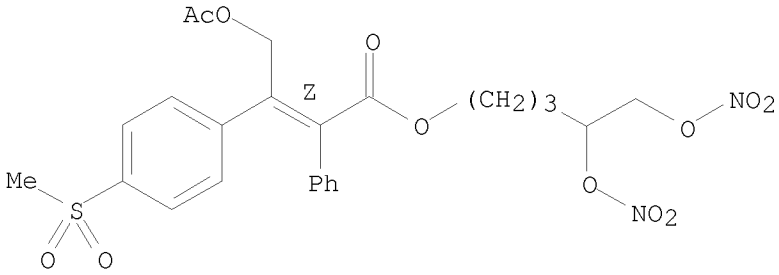
Absolute stereochemistry.
Double bond geometry as shown.



RN 861655-85-8 ZCAPLUS

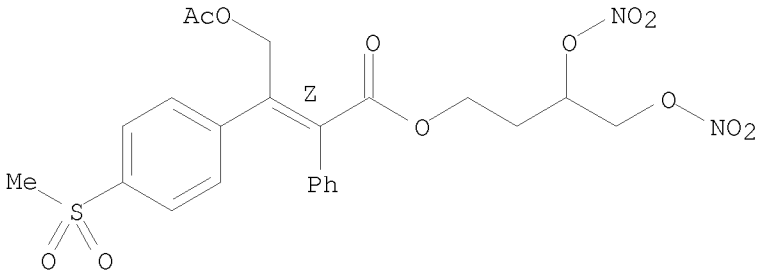
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 861655-86-9 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:739958 ZCAPLUS
DOCUMENT NUMBER: 141:260542
TITLE: Preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as selective cyclooxygenase-2 inhibitors
INVENTOR(S): Berthelette, Carl; Li, Lianhai; Sturino, Claudio; Wang, Zhaoyin
PATENT ASSIGNEE(S): Merck Frosst Company, Can.
SOURCE: U.S. Pat. Appl. Publ., 19 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040176331	A1	20040909	US 2004-790288	20040301
US 7169809	B2	20070130		
AU 2004240700	A1	20041202	AU 2004-240700	20040301
CA 2517490	A1	20041202	CA 2004-2517490	20040301
WO 2004103955	A1	20041202	WO 2004-CA314	20040301

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG

EP 1601644	A1	20051207	EP 2004-761562	20040301
EP 1601644	B1	20090527		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
JP 2007516954	T	20070628	JP 2006-529472	20040301
PRIORITY APPLN. INFO.:			US 2003-452124P P	20030305
			WO 2004-CA314 W	20040301

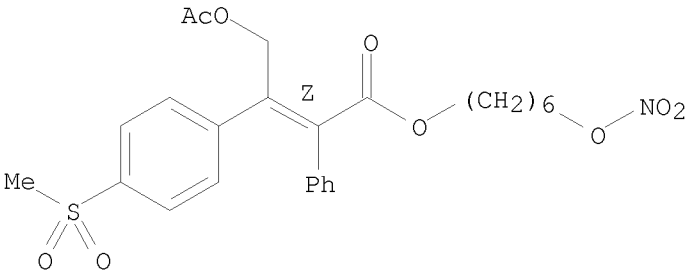
OTHER SOURCE(S): MARPAT 141:260542

IT 754241-98-0P 754241-99-1P 754242-00-7P
754242-01-8P 754242-02-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

RN 754241-98-0 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (αZ)- (CA INDEX NAME)

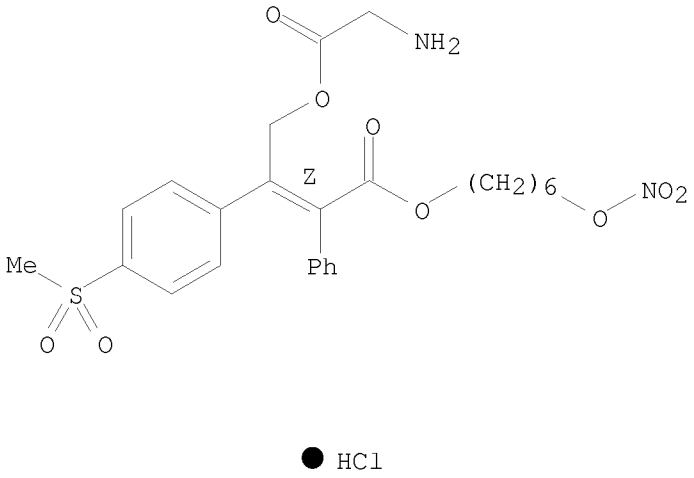
Double bond geometry as shown.



RN 754241-99-1 ZCAPLUS

CN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-butenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

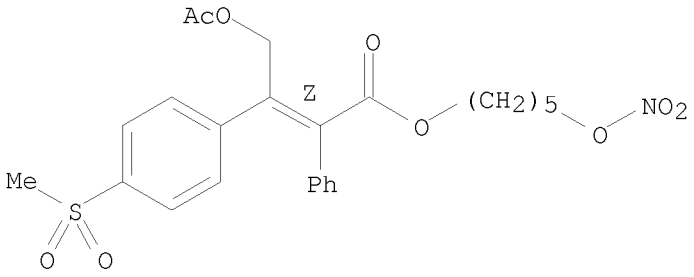
Double bond geometry as shown.



● HCl

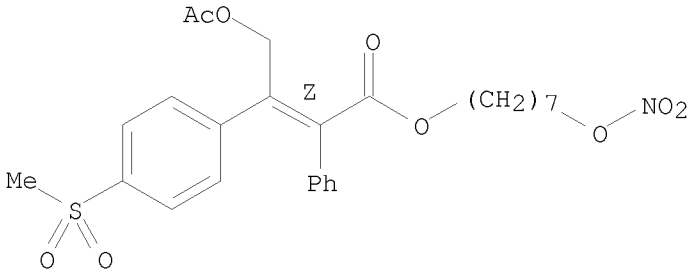
RN 754242-00-7 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5-(nitrooxy)pentyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



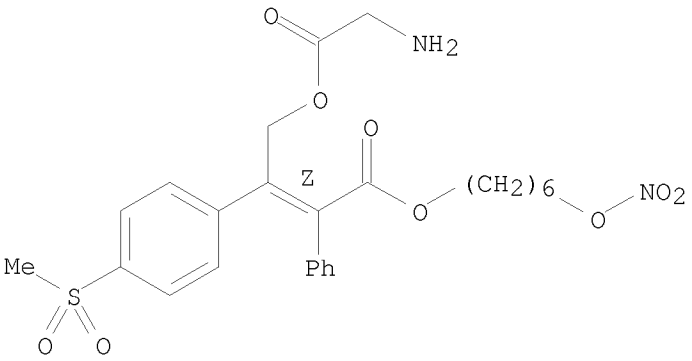
RN 754242-01-8 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 7-(nitrooxy)heptyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 754242-02-9 ZCAPLUS
CN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

Double bond geometry as shown.

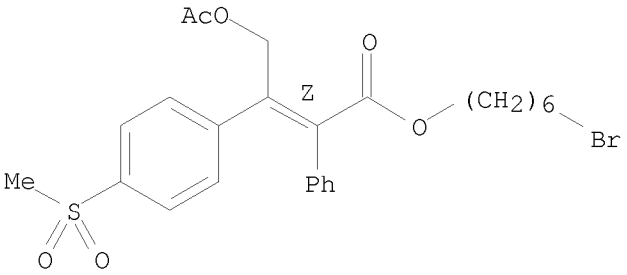


IT 754242-04-1P 754242-08-5P 754242-09-6P
754242-12-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

RN 754242-04-1 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (αZ)- (CA INDEX NAME)

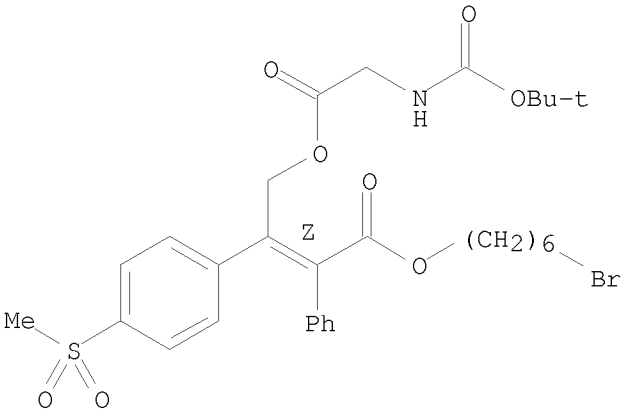
Double bond geometry as shown.



RN 754242-08-5 ZCAPLUS

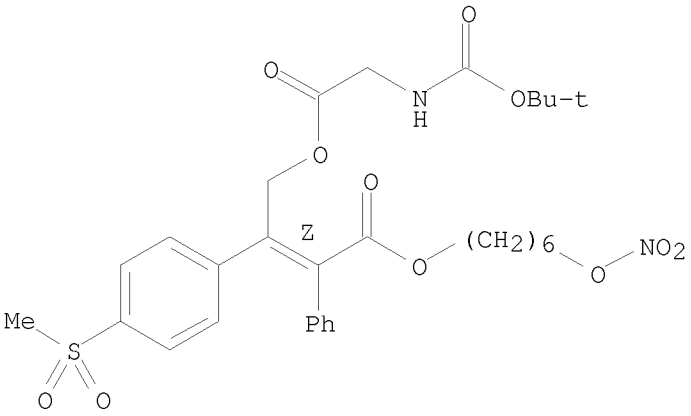
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (2Z)-4-[(6-bromohexyl)oxy]-2-[4-(methylsulfonyl)phenyl]-4-oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

Double bond geometry as shown.



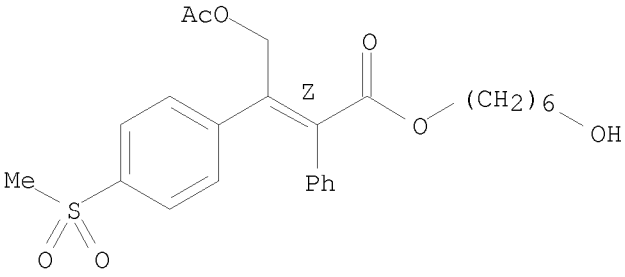
RN 754242-09-6 ZCAPLUS
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 754242-12-1 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (αZ)-(CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

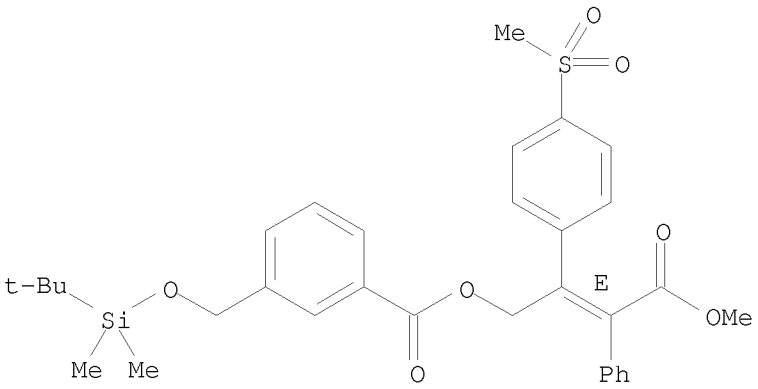
L9 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:101124 ZCAPLUS
DOCUMENT NUMBER: 140:163574
TITLE: Preparation of nitric oxide releasing diaryl-2-(5H)-furanone prodrugs as selective cyclooxygenase-2 inhibitors for treatment inflammatory diseases
INVENTOR(S): Berthelette, Carl; Lachance, Nicholas; Li, Lianhai; Sturino, Claudio; Wang, Zhaoyin; Young, Robert N.; Dufresne, Claude
PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011421	A1	20040205	WO 2003-CA1115	20030724
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2493082	A1	20040205	CA 2003-2493082	20030724
AU 2003252515	A1	20040216	AU 2003-252515	20030724
EP 1527045	A1	20050504	EP 2003-771010	20030724
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 20050261245	A1	20051124	US 2005-521075	20050112
US 7199154	B2	20070403		

PRIORITY APPLN. INFO.:	US 2002-398683P	P	20020726
	US 2002-435341P	P	20021220
	WO 2003-CA1115	W	20030724

OTHER SOURCE(S): CASREACT 140:163574; MARPAT 140:163574
IT 654069-14-4P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of nitric oxide releasing diarylfuranone prodrugs as selective cyclooxygenase-2 inhibitors for treatment of inflammatory diseases)
RN 654069-14-4 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αE)- (CA INDEX NAME)

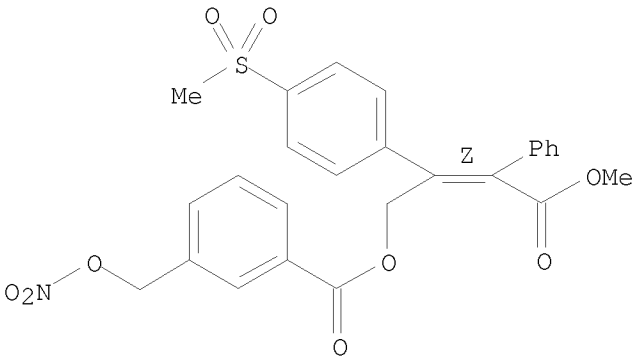
Double bond geometry as shown.



IT 654068-75-4P 654068-76-5P 654068-79-8P
654068-81-2P 654068-83-4P 654068-84-5P
654068-85-6P 654068-86-7P 654068-87-8P
654068-88-9P 654068-89-0P 654068-90-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing diarylfuranone prodrugs as selective cyclooxygenase-2 inhibitors for treatment of inflammatory diseases)

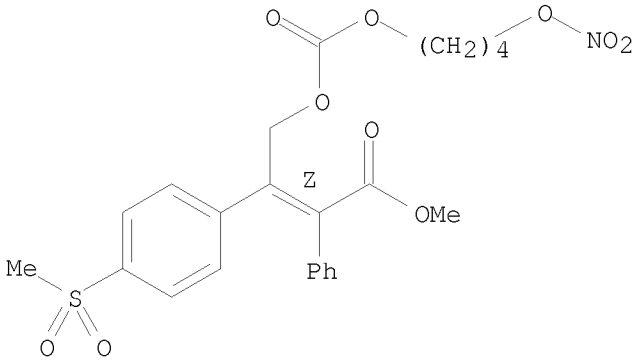
RN 654068-75-4 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[3-[(nitrooxy)methyl]benzoyl]oxy]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



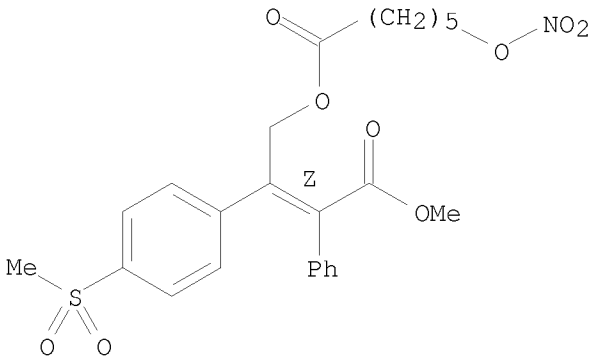
RN 654068-76-5 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



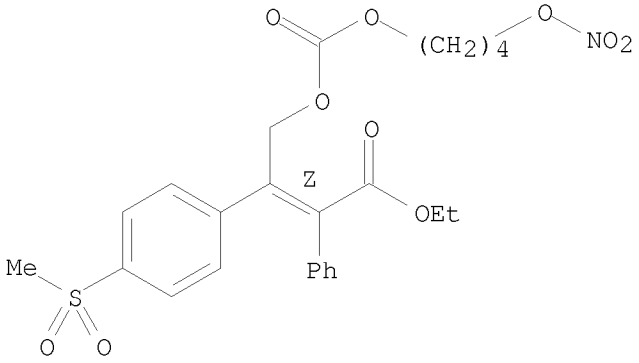
RN 654068-79-8 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 654068-81-2 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, ethyl ester, (αZ)- (CA INDEX NAME)

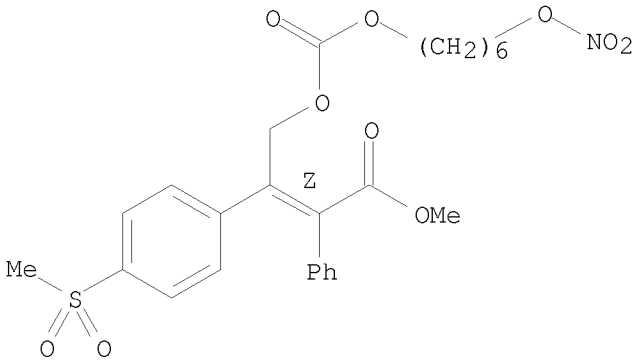
Double bond geometry as shown.



RN 654068-83-4 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (αZ)-

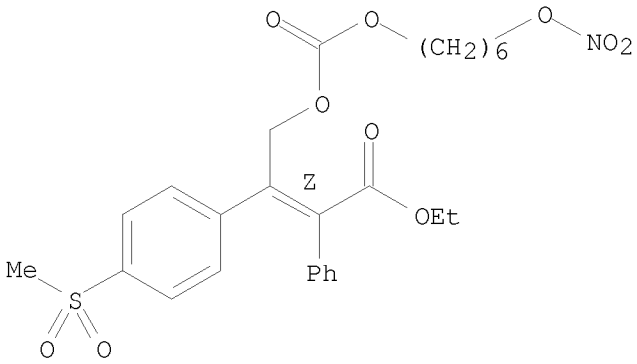
(CA INDEX NAME)

Double bond geometry as shown.



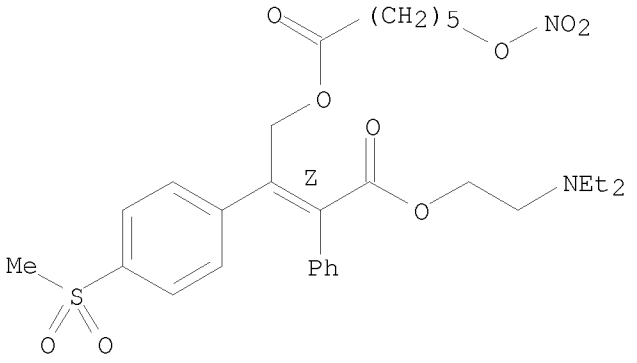
RN 654068-84-5 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



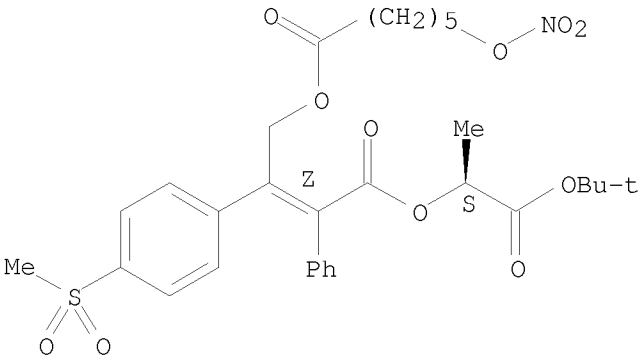
RN 654068-85-6 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



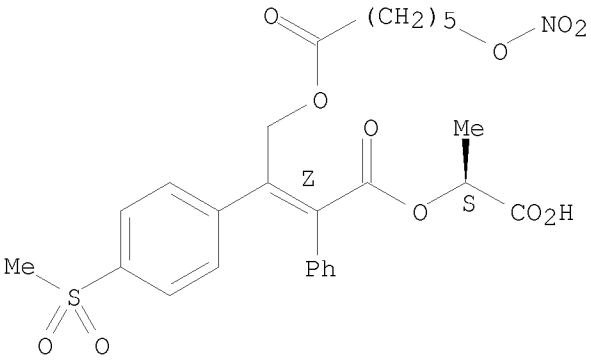
RN 654068-86-7 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl ester, (αZ)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



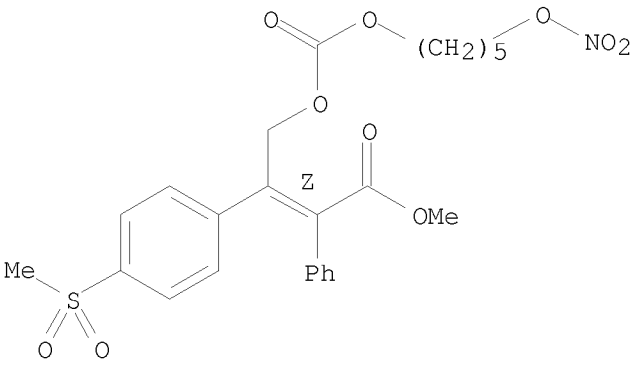
RN 654068-87-8 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-1-carboxyethyl ester, (αZ)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



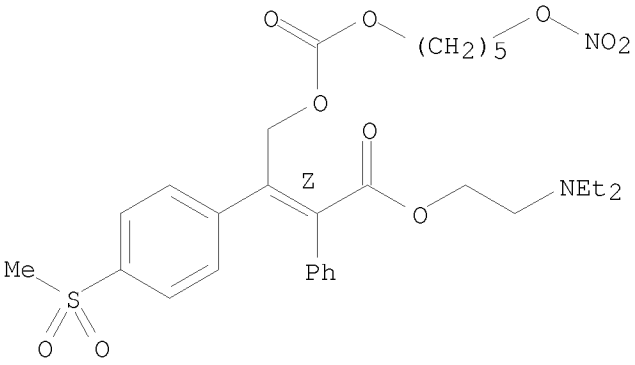
RN 654068-88-9 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 654068-89-0 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, hydrochloride (1:1), (αZ)- (CA INDEX NAME)

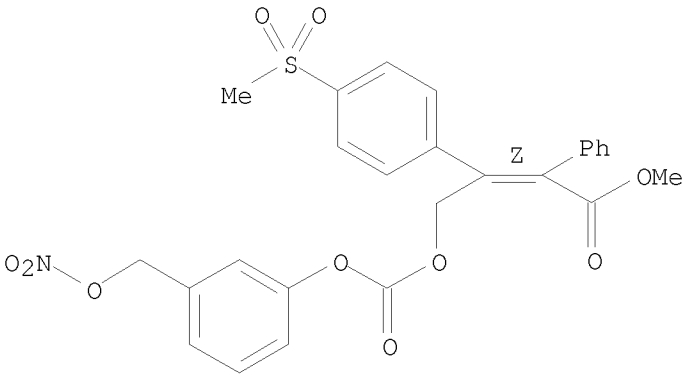
Double bond geometry as shown.



● HCl

RN 654068-90-3 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[3-[(nitrooxy)methyl]phenoxy]carbonyl]oxy]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

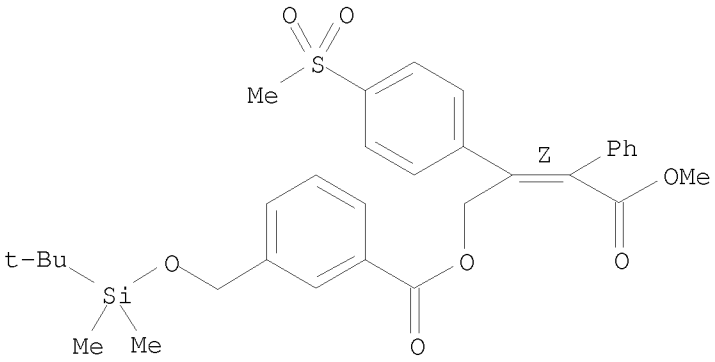
Double bond geometry as shown.



IT 654068-91-4P 654068-95-8P 654068-98-1P
654069-03-1P 654069-09-7P 654069-10-0P
654069-11-1P 654069-15-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitric oxide releasing diarylfuranone prodrugs as selective cyclooxygenase-2 inhibitors for treatment of inflammatory diseases)

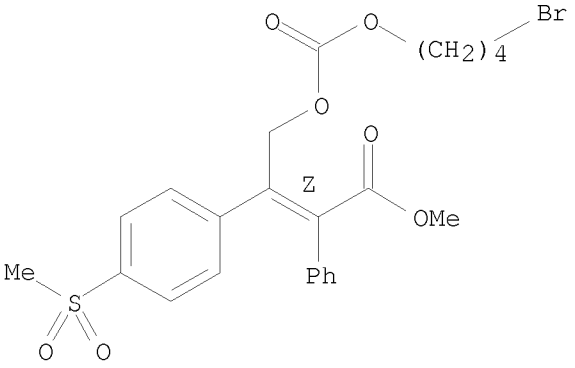
RN 654068-91-4 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



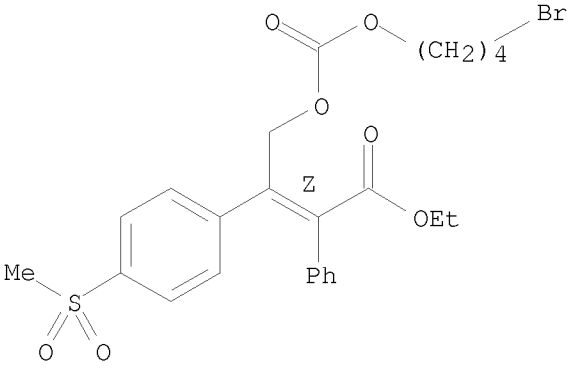
RN 654068-95-8 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



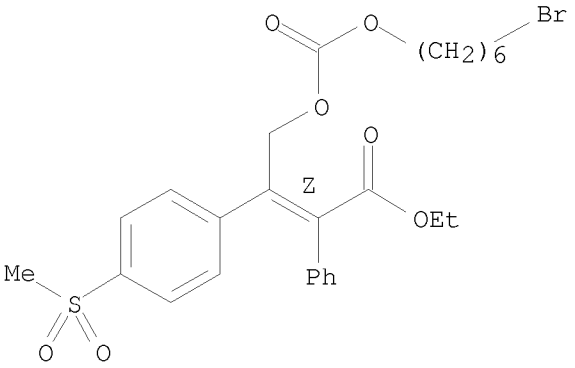
RN 654068-98-1 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 654069-03-1 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)- (CA INDEX NAME)

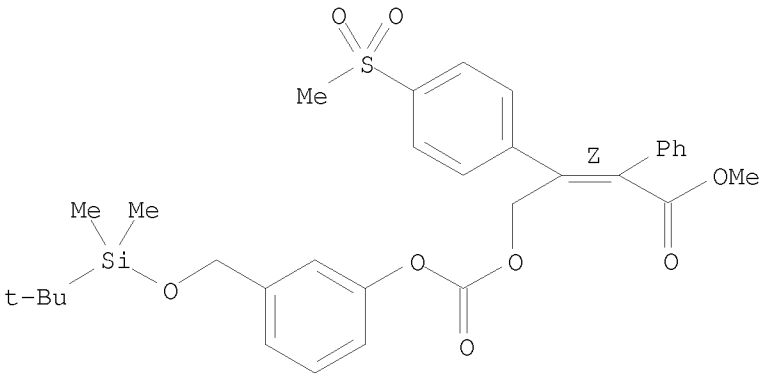
Double bond geometry as shown.



RN 654069-09-7 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[[3-[[[(1,1-

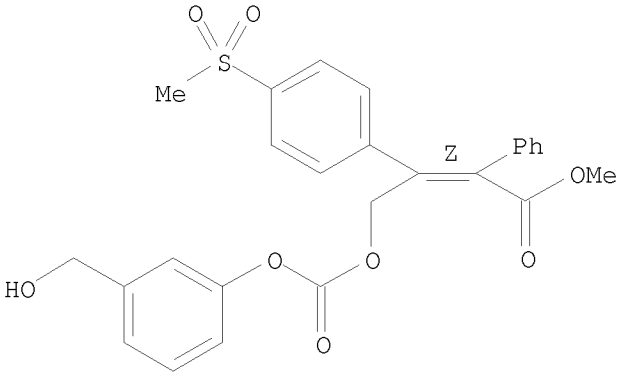
dimethylethyl)dimethylsilyl]oxy]methyl]phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



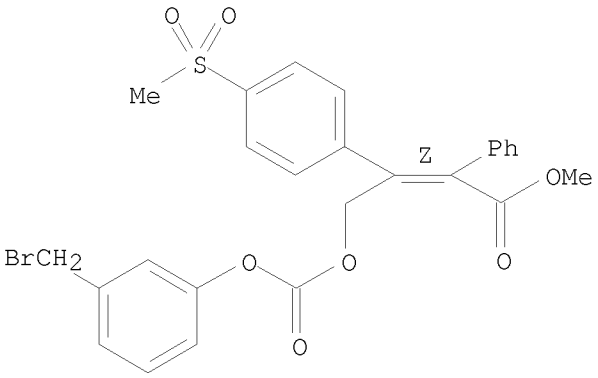
RN 654069-10-0 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[[3-(hydroxymethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



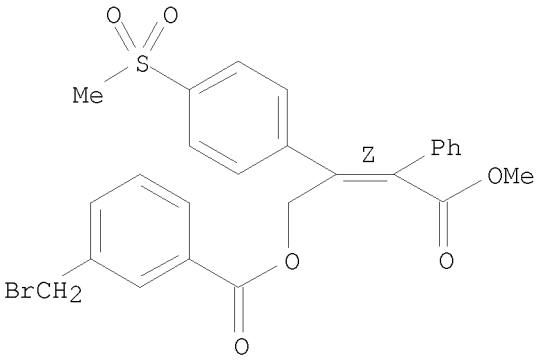
RN 654069-11-1 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[[3-(bromomethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 654069-15-5 ZCAPLUS
CN Benzeneacetic acid, α-[2-[[3-(bromomethyl)benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:472491 ZCAPLUS
DOCUMENT NUMBER: 135:76524
TITLE: Preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors
INVENTOR(S): Bandarage, Ramani R.; Bandarage, Upul K.; Fang, Xinqin; Garvey, David S.; Letts, L. Gordon; Schroeder, Joseph D.; Tam, Sang William
PATENT ASSIGNEE(S): Nitromed, Inc., USA
SOURCE: PCT Int. Appl., 230 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001045703	A1	20010628	WO 2000-US35014	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,				

HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2393724	A1	20010628	CA 2000-2393724	20001222
US 20010041726	A1	20011115	US 2000-741816	20001222
US 6649629	B2	20031118		
EP 1246621	A1	20021009	EP 2000-989422	20001222
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2000017037	A	20030610	BR 2000-17037	20001222
JP 2003523958	T	20030812	JP 2001-546642	20001222
NZ 519781	A	20040430	NZ 2000-519781	20001222
AU 782971	B2	20050915	AU 2001-25928	20001222
MX 2002006312	A	20040621	MX 2002-6312	20020624
ZA 2002005707	A	20031111	ZA 2002-5707	20020717
US 20030220228	A1	20031127	US 2003-463671	20030618
US 7166618	B2	20070123		
US 20070060571	A1	20070315	US 2006-599519	20061115
US 7432285	B2	20081007		
US 20090099139	A1	20090416	US 2008-196184	20080821

PRIORITY APPLN. INFO.:	US 1999-171623P	P	19991223
	US 2000-226085P	P	20000818
	US 2000-741816	A3	20001222
	WO 2000-US35014	W	20001222
	US 2003-463671	A3	20030618
	US 2006-599519	A3	20061115

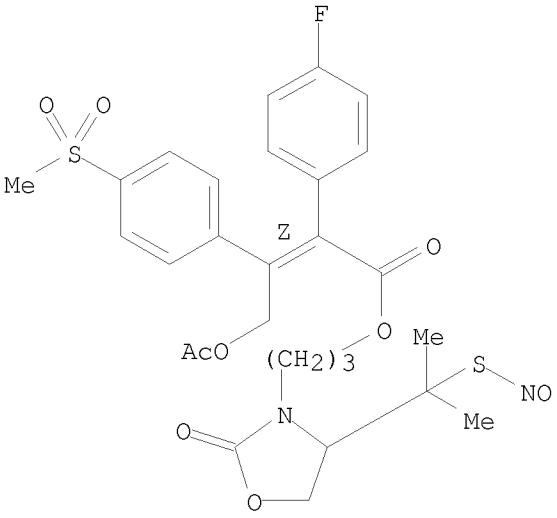
OTHER SOURCE(S): MARPAT 135:76524

IT 346683-81-6P 346683-83-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrosated and nitrosylated cyclooxygenase-2 inhibitors)

RN 346683-81-6 ZCAPLUS

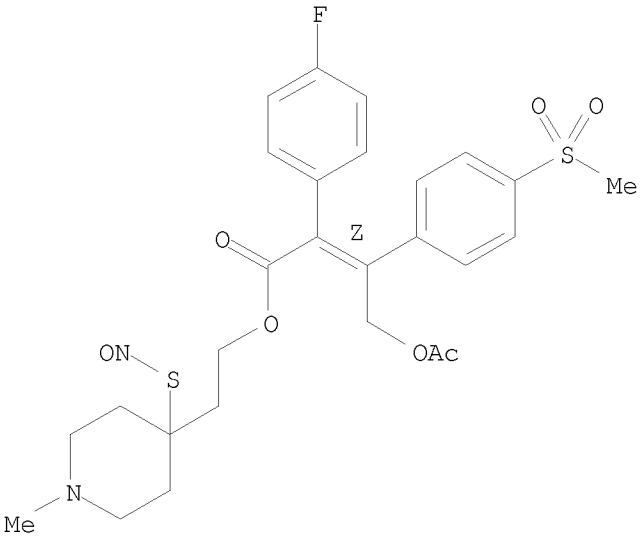
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 3-[4-[1-methyl-1-(nitrosothio)ethyl]-2-oxo-3-oxazolidinyl]propyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 346683-83-8 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:462317 ZCAPLUS
DOCUMENT NUMBER: 125:114294
ORIGINAL REFERENCE NO.: 125:21435a,21438a
TITLE: Preparation of stilbene derivatives useful as cyclooxygenase-2 inhibitors
INVENTOR(S): Atkinson, Joseph G.; Wang, Zhaoyin
PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.
SOURCE: PCT Int. Appl., 80 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9613483	A1	19960509	WO 1995-CA601	19951024
W: AL, AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2200462	A1	19960509	CA 1995-2200462	19951024
AU 9536950	A	19960523	AU 1995-36950	19951024
AU 688980	B2	19980319		
EP 788476	A1	19970813	EP 1995-944787	19951024
EP 788476	B1	19991020		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 10507765	T	19980728	JP 1995-514204	19951024
AT 185797	T	19991115	AT 1995-944787	19951024
ES 2139959	T3	20000216	ES 1995-944787	19951024
US 5849943	A	19981215	US 1997-817128	19970407

PRIORITY APPLN. INFO.: US 1994-330172 A1 19941027
WO 1995-CA601 W 19951024

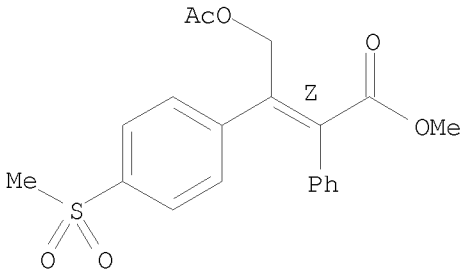
OTHER SOURCE(S): MARPAT 125:114294

IT 179174-84-6P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of stilbene derivs. useful as cyclooxygenase-2 inhibitors)

RN 179174-84-6 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

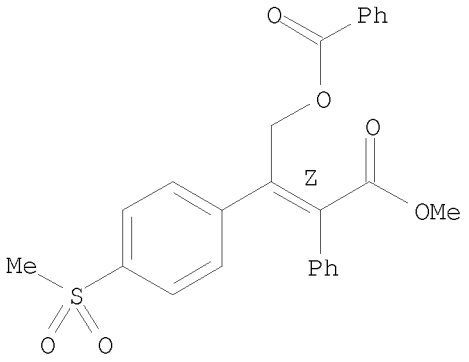


IT 179174-89-1 179174-90-4 179174-95-9
179175-00-9 179175-04-3 179175-09-8
179175-14-5
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of stilbene derivs. useful as cyclooxygenase-2 inhibitors)

RN 179174-89-1 ZCAPLUS

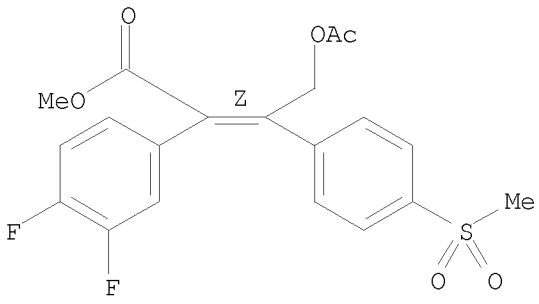
CN Benzeneacetic acid, α-[2-(benzoyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



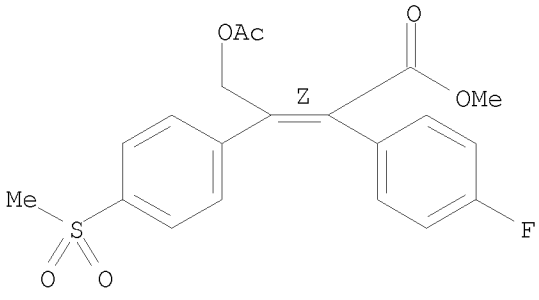
RN 179174-90-4 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



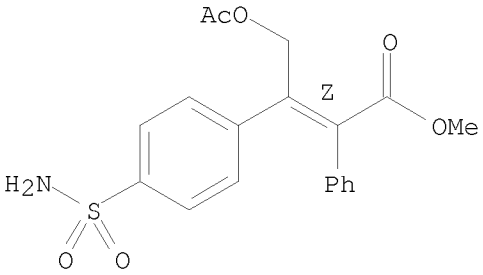
RN 179174-95-9 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



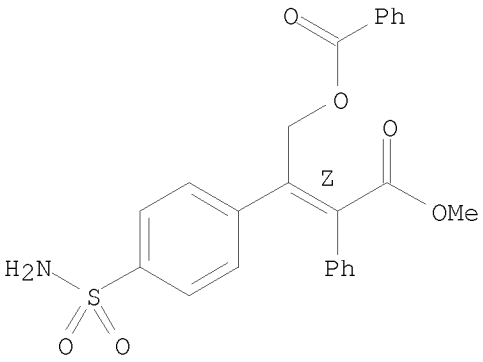
RN 179175-00-9 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



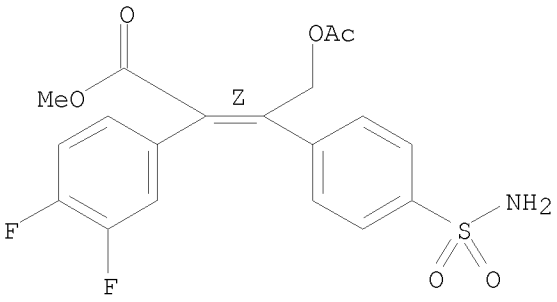
RN 179175-04-3 ZCAPLUS
CN Benzeneacetic acid, α-[1-[4-(aminosulfonyl)phenyl]-2-(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



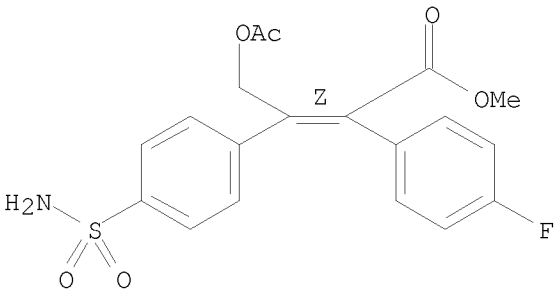
RN 179175-09-8 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 179175-14-5 ZCAPLUS
CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 10:54:15 ON 17 JUN 2009)

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 17 JUN 2009
L1 STRUCTURE UPLOADED
L2 4 S SAM SSS L1
L3 84 S FULL SSS L1

FILE 'ZCAPLUS' ENTERED AT 11:14:23 ON 17 JUN 2009
E US2006-586573/APPS
L4 1 S US2006-586573/APPS
SEL RN

FILE 'REGISTRY' ENTERED AT 11:15:49 ON 17 JUN 2009
L5 34 S E1-E34
L6 4 S L3 AND L5

FILE 'ZCAPLUS' ENTERED AT 11:18:58 ON 17 JUN 2009
L7 18 S L3
L8 1 S L7 AND (NITROSATED OR NITROSYLATED)
L9 11 S L7 AND (NITROSATED OR NITROSYLATED OR NO OR (NITRIC (W) OXIDE

=> exit
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	67.29	277.05

STN INTERNATIONAL LOGOFF AT 11:59:21 ON 17 JUN 2009

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAVXR1614

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  DEC 01  ChemPort single article sales feature unavailable
 NEWS  3  APR 03  CAS coverage of exemplified prophetic substances
                  enhanced
 NEWS  4  APR 07  STN is raising the limits on saved answers
 NEWS  5  APR 24  CA/CAplus now has more comprehensive patent assignee
                  information
 NEWS  6  APR 26  USPATFULL and USPAT2 enhanced with patent
                  assignment/reassignment information
 NEWS  7  APR 28  CAS patent authority coverage expanded
 NEWS  8  APR 28  ENCOMPLIT/ENCOMPLIT2 search fields enhanced
 NEWS  9  APR 28  Limits doubled for structure searching in CAS
                  REGISTRY
 NEWS 10  MAY 08  STN Express, Version 8.4, now available
 NEWS 11  MAY 11  STN on the Web enhanced
 NEWS 12  MAY 11  BEILSTEIN substance information now available on
                  STN Easy
 NEWS 13  MAY 14  DGENE, PCTGEN and USGENE enhanced with increased
                  limits for exact sequence match searches and
                  introduction of free HIT display format
 NEWS 14  MAY 15  INPADOCDB and INPAFAMDB enhanced with Chinese legal
                  status data
 NEWS 15  MAY 28  CAS databases on STN enhanced with NANO super role in
                  records back to 1992
 NEWS 16  JUN 01  CAS REGISTRY Source of Registration (SR) searching
                  enhanced on STN
 NEWS 17  JUN 26  NUTRACEUT and PHARMAML no longer updated

 NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
              AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
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Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:40:52 ON 29 JUN 2009

=>  file registry
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.22       0.22

FILE 'REGISTRY' ENTERED AT 09:41:02 ON 29 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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```

Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 28 JUN 2009 HIGHEST RN 1160218-33-6
DICTIONARY FILE UPDATES: 28 JUN 2009 HIGHEST RN 1160218-33-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

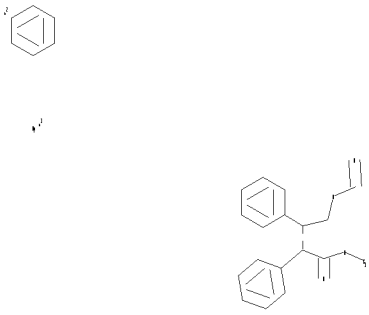
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

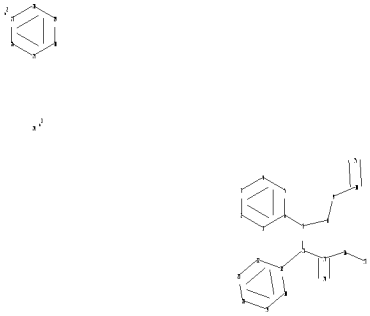
  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red
Folder\10586573\L1-1.str





chain nodes :
7 8 9 10 11 13 14 15 16 17 24
ring nodes :

```
1  2  3  4  5  6  12  18  19  20  21  22  25  26  27  28  29  30
chain bonds :
6-7  7-8  7-11  8-9  9-10  10-15  11-12  11-13  13-14  13-16  16-17
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-18  12-22  18-19  19-20  20-21  21-22  25-26
25-30  26-27  27-28  28-29  29-30
exact/norm bonds :
7-11  8-9  9-10  10-15  13-14  13-16  16-17
exact bonds :
6-7  7-8  11-12  11-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-18  12-22  18-19  19-20  20-21  21-22  25-26
25-30  26-27  27-28  28-29  29-30
isolated ring systems :
containing 1 : 12 :


G1:H,[*1],[*2]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
 11:CLASS  12:Atom  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:Atom
19:Atom  20:Atom  21:Atom  22:Atom  24:Atom  25:Atom  26:Atom  27:Atom  28:Atom
29:Atom  30:Atom



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s sam l1
SAMPLE SEARCH INITIATED 09:41:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       29 TO ITERATE

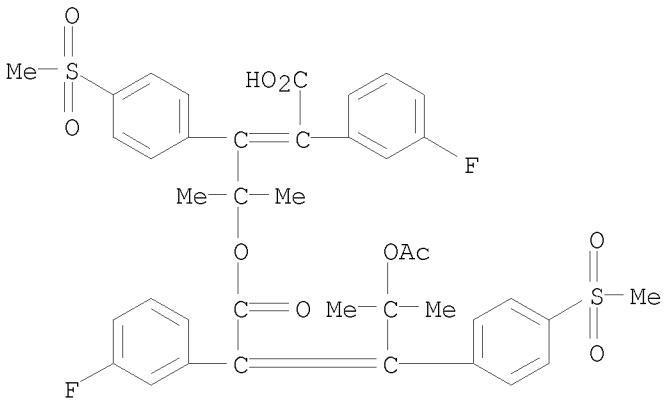
100.0% PROCESSED       29 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          257 TO      903
PROJECTED ANSWERS:               3 TO      163

L2            3 SEA SSS SAM L1

=> d sca

L2   3 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-
     3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-
     (methylsulfonyl)phenyl]propylidene]-3-fluoro-
MF   C40 H38 F2 O10 S2
CI   COM
```

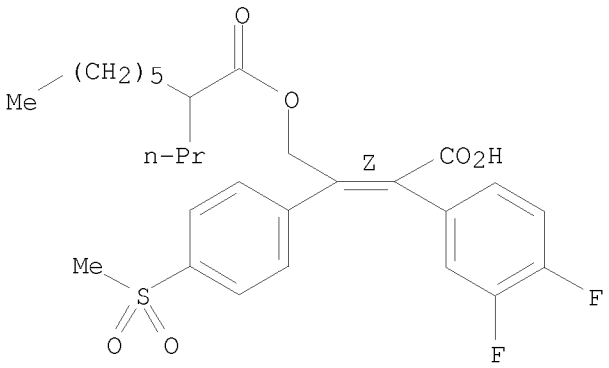


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, 3,4-difluoro-α-[1-[4-(methylsulfonyl)phenyl]-2-[(1-oxo-2-propyloctyl)oxy]ethylidene]-, (αZ)-
MF C28 H34 F2 O6 S

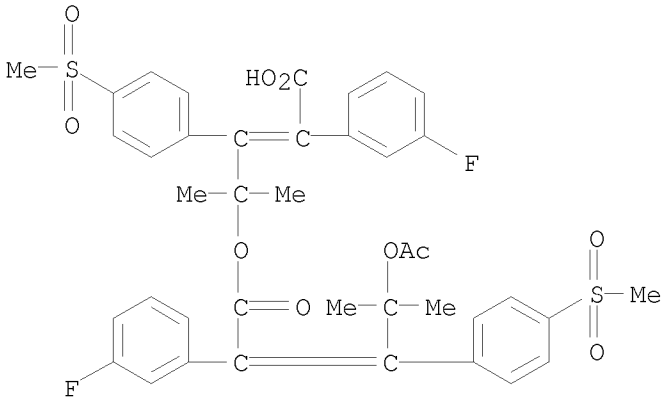
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, sodium salt (1:1)
MF C40 H38 F2 O10 S2 . Na



● Na

ALL ANSWERS HAVE BEEN SCANNED

```
=> s full sss l1
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:42:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      767 TO ITERATE

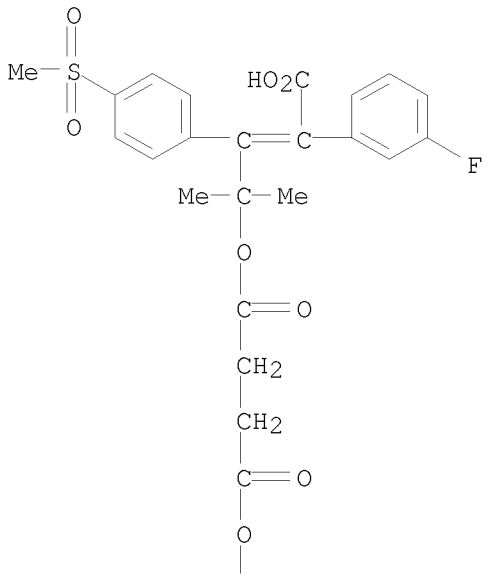
100.0% PROCESSED      767 ITERATIONS                                51 ANSWERS
SEARCH TIME: 00.00.01

L3           51 SEA SSS FUL L1

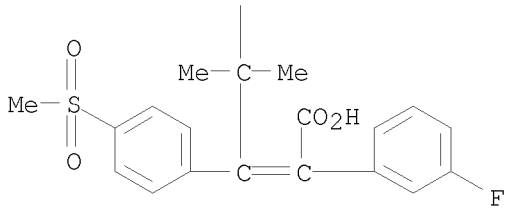
=> d sca

L3   51 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   Butanedioic acid, 1,4-bis[3-carboxy-3-(3-fluorophenyl)-1,1-dimethyl-2-[4-
     (methylsulfonyl)phenyl]-2-propen-1-yl] ester
MF   C42 H40 F2 O12 S2
CI   COM
```

PAGE 1-A



PAGE 2-A

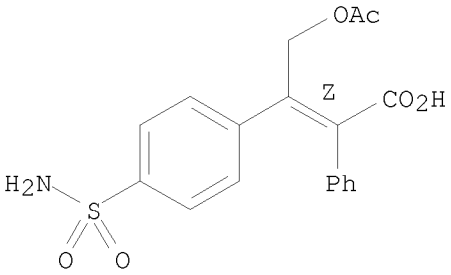


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-, (Z)- (9CI)
MF C18 H17 N O6 S

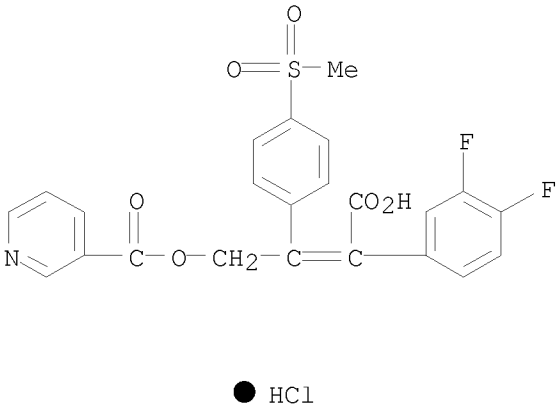
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

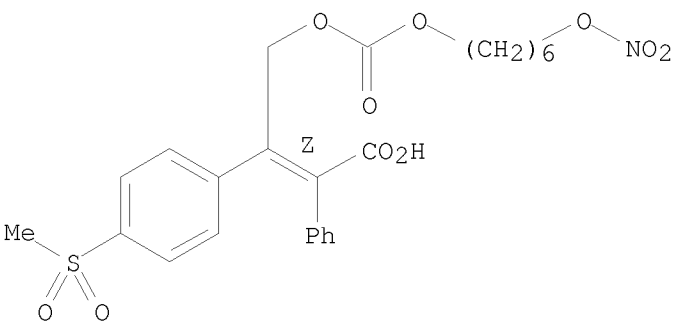
L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 3-Pyridinecarboxylic acid, 3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl ester, hydrochloride (1:1)
MF C23 H17 F2 N O6 S . Cl H



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, (αZ)-
MF C24 H27 N O10 S

Double bond geometry as shown.

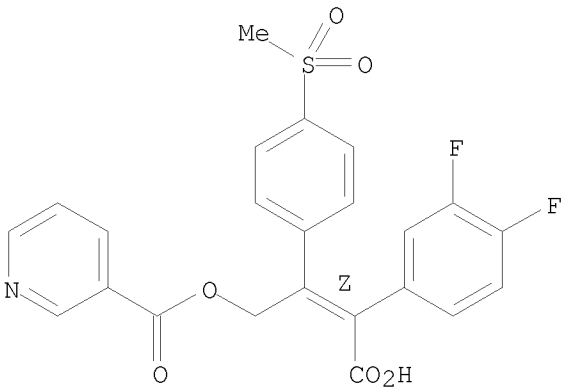


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 3-Pyridinecarboxylic acid, (2Z)-3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl ester
MF C23 H17 F2 N O6 S

Double bond geometry as shown.

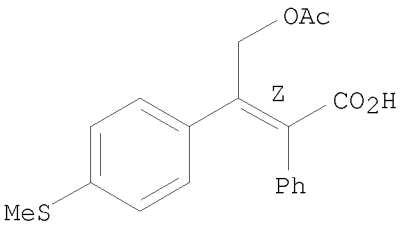


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylthio)phenyl]ethylidene]-, magnesium salt, hydrate (2:1:?), (αZ)-
MF C19 H18 O4 S . x H2 O . 1/2 Mg

Double bond geometry as shown.



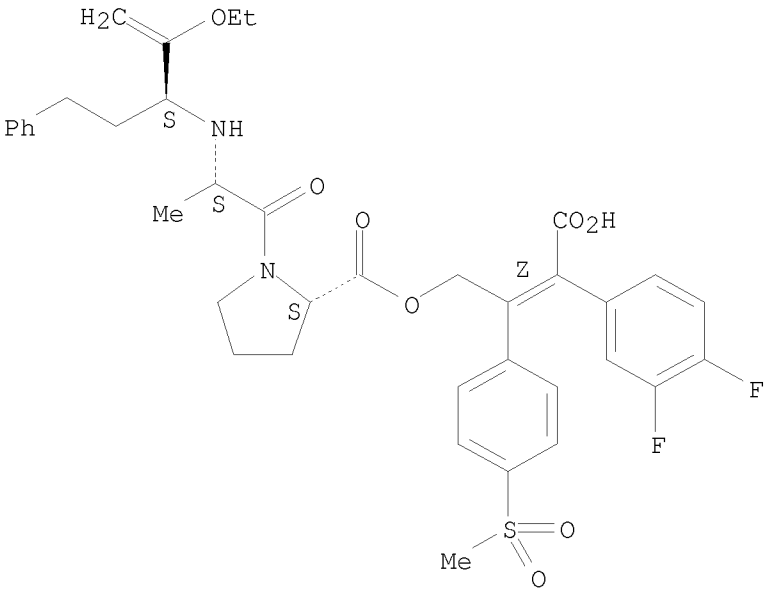
●1/2 Mg

●x H2O

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN L-Proline, N-[(1S)-2-ethoxy-1-(2-phenylethyl)-2-propenyl]-L-alanyl-, (2Z)-3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propenyl ester (9CI)
MF C38 H42 F2 N2 O8 S

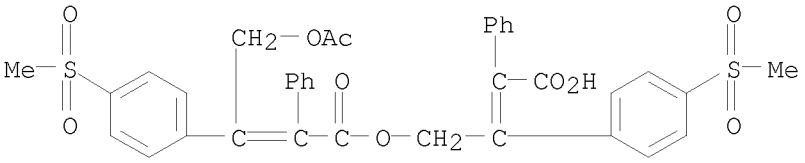
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

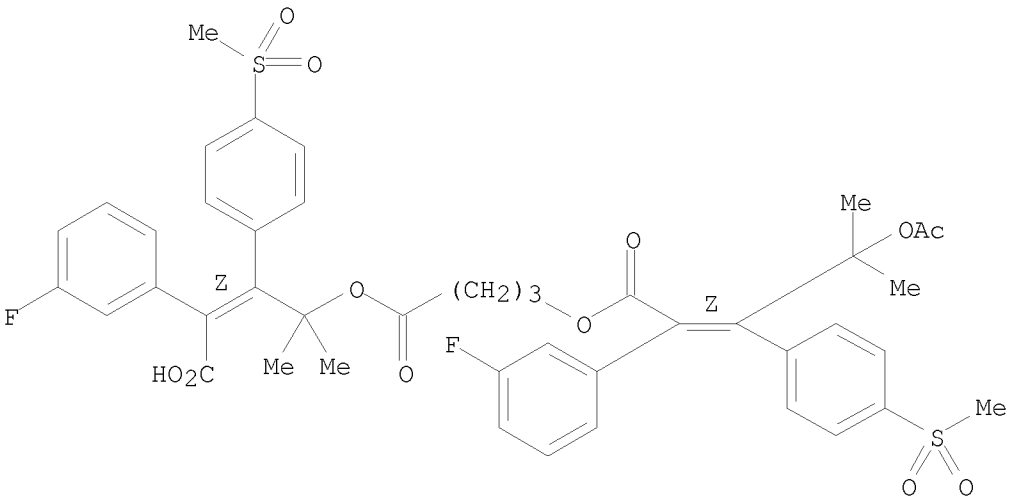
L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
    (methylsulfonyl)phenyl]ethylidene]-,
    3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester,
    sodium salt (1:1)
MF C36 H32 O10 S2 . Na



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[4-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-
    4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-1-
    oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-,
    (αZ)-
MF C44 H44 F2 O12 S2
CI COM

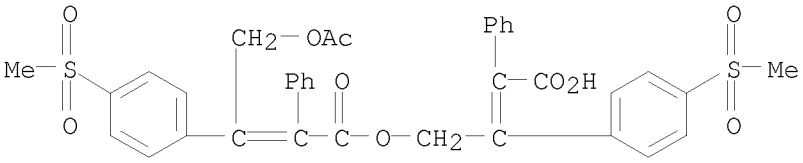
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
    (methylsulfonyl)phenyl]ethylidene]-,
    3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester
MF C36 H32 O10 S2
CI COM

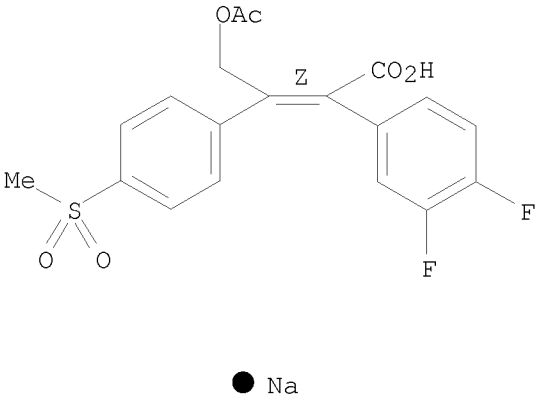


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
    (methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, sodium salt, (Z)- (9CI)
MF C19 H16 F2 O6 S . Na

Double bond geometry as shown.

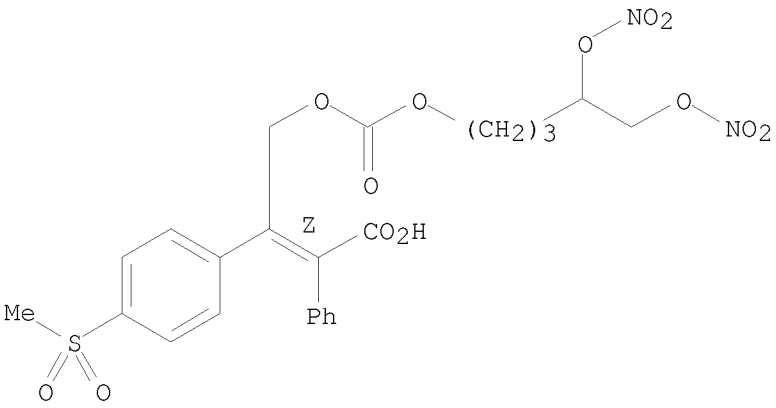


● Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[[4,5-
    bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-
    (methylsulfonyl)phenyl]ethylidene]-, (αZ)-
MF C23 H24 N2 O13 S

Double bond geometry as shown.

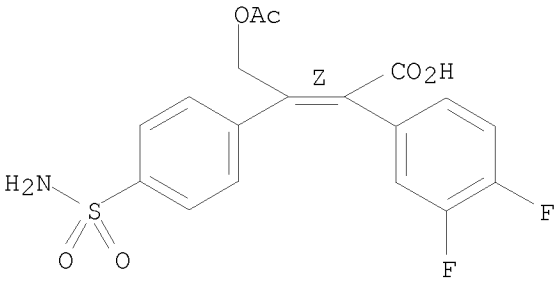


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, (Z)- (9CI)
MF C18 H15 F2 N O6 S

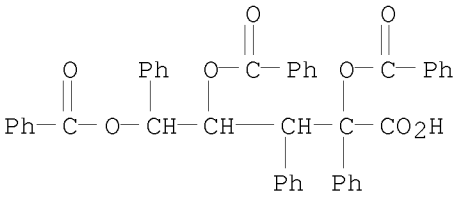
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Valeric acid, α,γ,δ-trihydroxy-α,β,δ-triphenyl-, tribenzoate (2CI)
MF C44 H34 O8

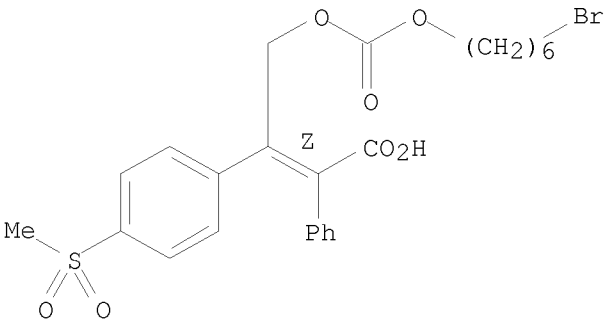


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (αZ)-
MF C24 H27 Br O7 S

Double bond geometry as shown.

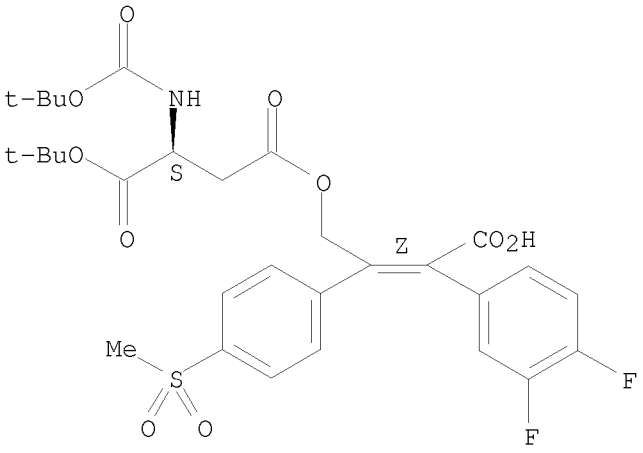


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN L-Aspartic acid, N-[(1,1-dimethylethoxy)carbonyl]-, 4-[(2Z)-3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl] 1-(1,1-dimethylethyl) ester
MF C30 H35 F2 N O10 S

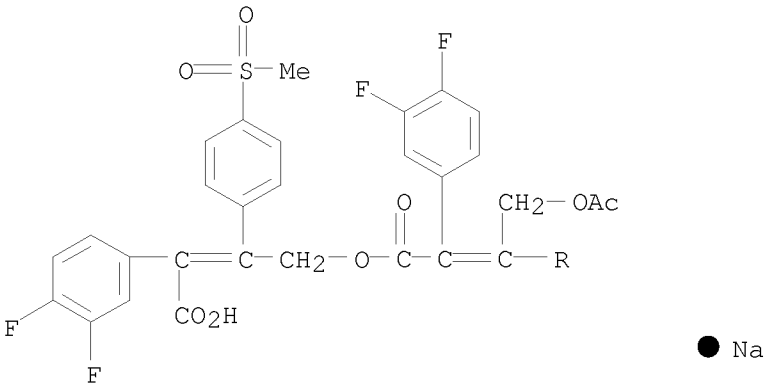
Absolute stereochemistry.
Double bond geometry as shown.

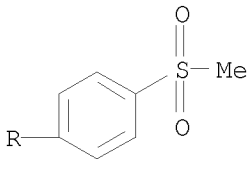


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, sodium salt (1:1)
MF C36 H28 F4 O10 S2 . Na



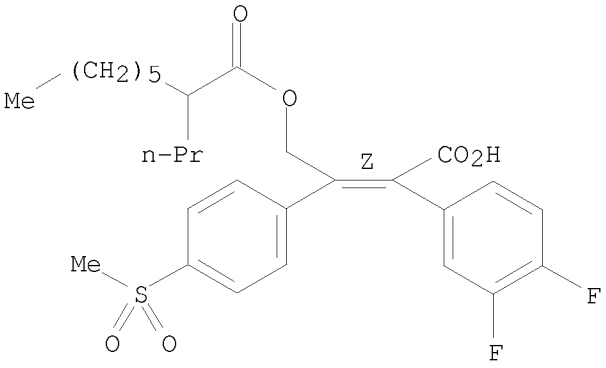


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, 3,4-difluoro-α-[1-[4-(methylsulfonyl)phenyl]-2-[(1-oxo-2-propyloctyl)oxy]ethylidene]-, (αZ)-

MF C28 H34 F2 O6 S

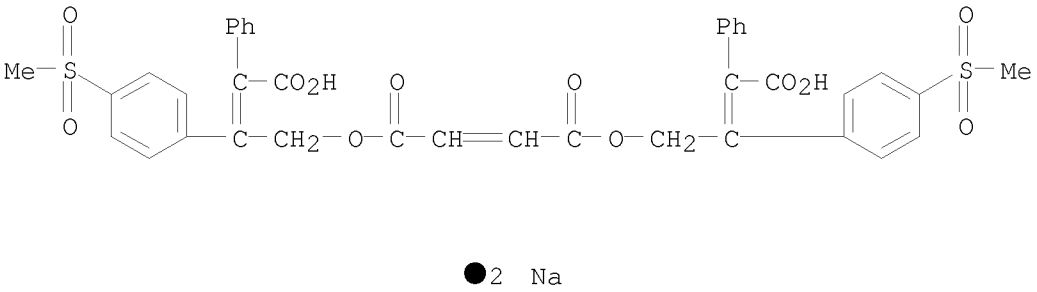
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

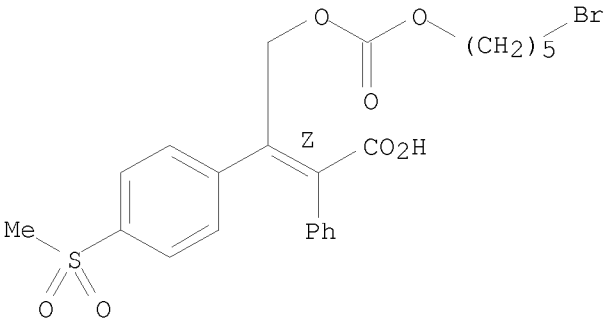
L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Butenedioic acid, bis[3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propenyl] ester, disodium salt (9CI)
MF C38 H32 O12 S2 . 2 Na



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C23 H25 Br O7 S

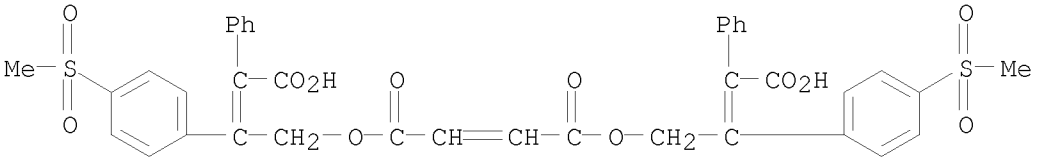
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Butenedioic acid, bis[3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propenyl] ester (9CI)
MF C38 H32 O12 S2
CI COM

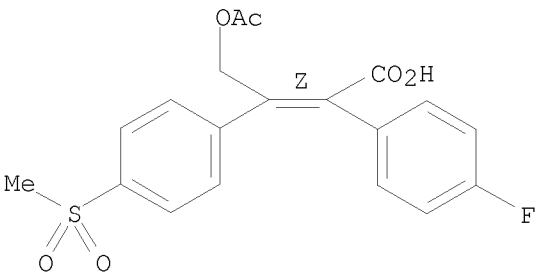


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, (αZ)-
MF C19 H17 F O6 S

Double bond geometry as shown.

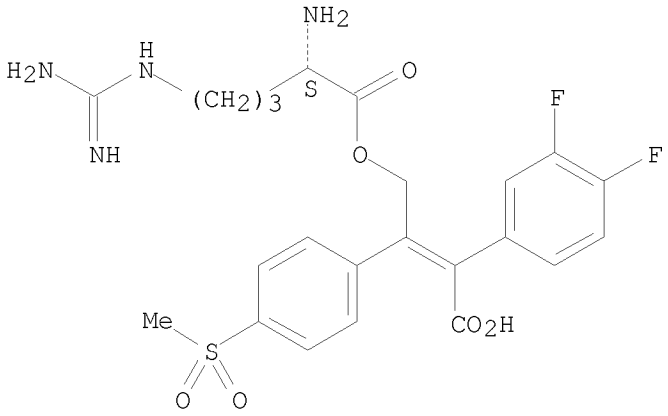


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[(2S)-2-amino-5-[(aminoiminomethyl)amino]-1-oxopentyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-(9CI)
MF C23 H26 F2 N4 O6 S

Absolute stereochemistry.
Double bond geometry unknown.

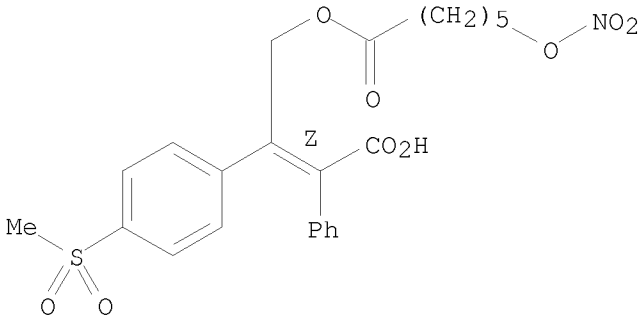


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (αZ)-
MF C23 H25 N O9 S

Double bond geometry as shown.

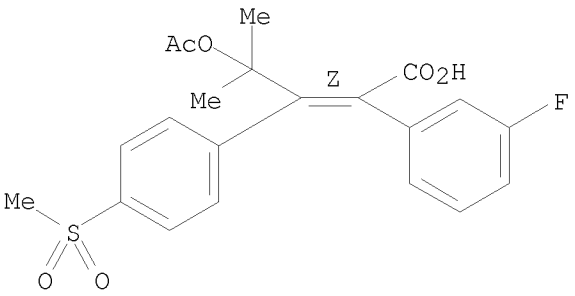


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, (αZ)-
MF C21 H21 F O6 S

Double bond geometry as shown.

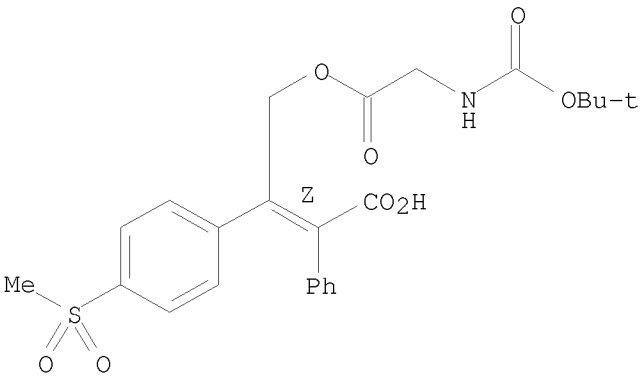


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (2Z)-3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester
MF C24 H27 N O8 S

Double bond geometry as shown.

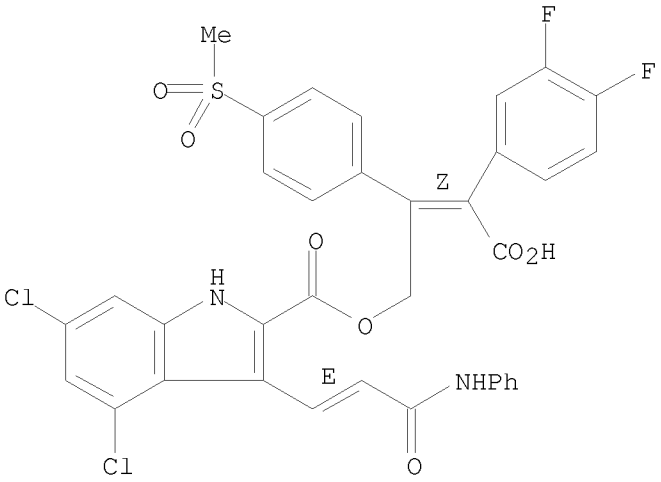


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Indole-2-carboxylic acid, 4,6-dichloro-3-[(1E)-3-oxo-3-(phenylamino)-1-propen-1-yl]-, (2Z)-3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl ester
MF C35 H24 Cl2 F2 N2 O7 S

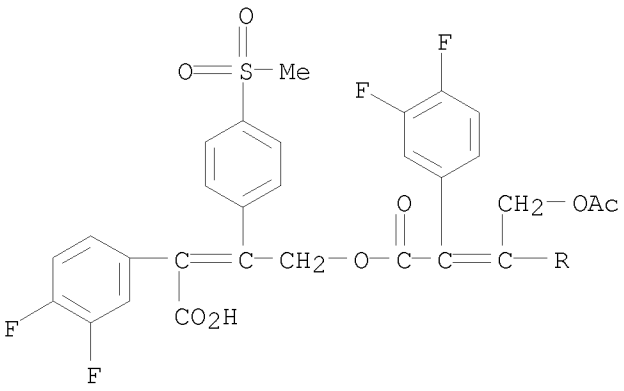
Double bond geometry as shown.

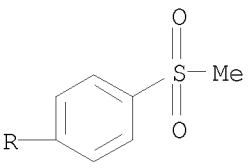


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-
MF C36 H28 F4 O10 S2
CI COM



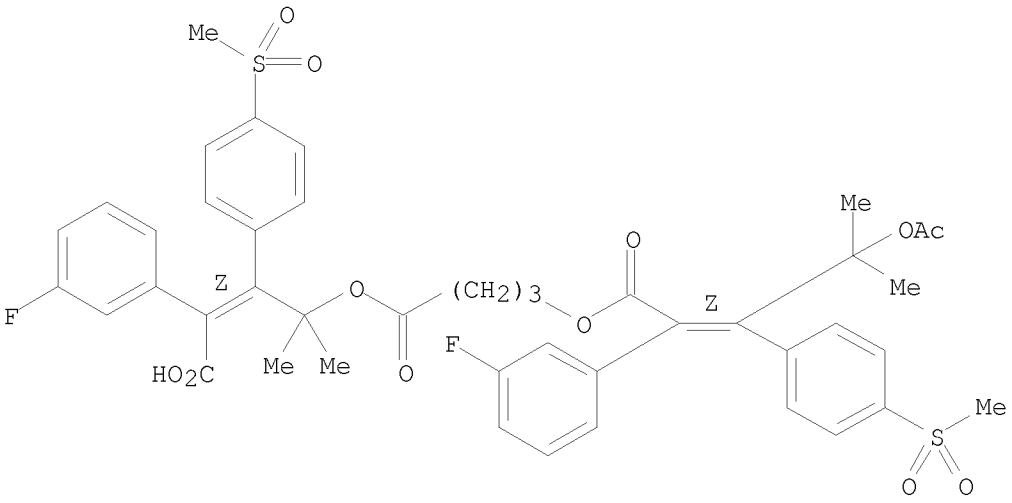


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C44 H44 F2 O12 S2 . Na

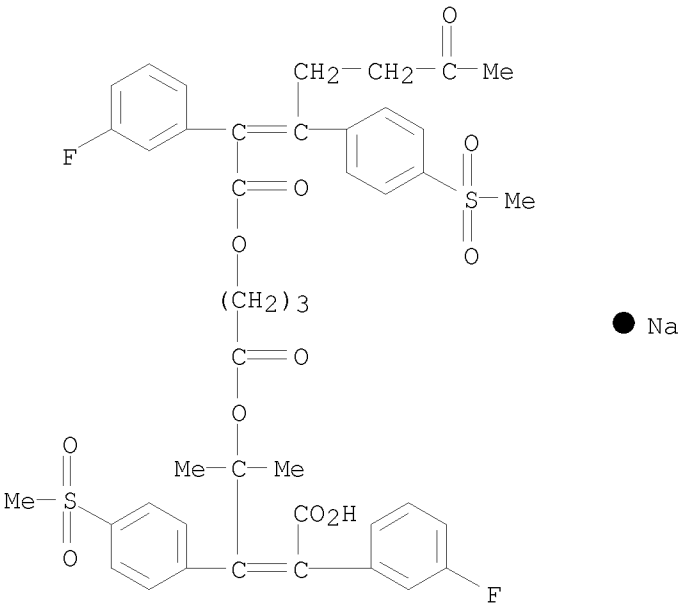
Double bond geometry as shown.



● Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

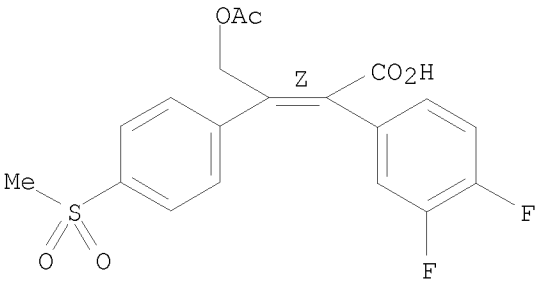
L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, 3-fluoro-α-[2-[4-[[2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1,6-dioxo-2-hepten-1-yl]oxy]-1-oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-, sodium salt (1:1)
MF C43 H42 F2 O11 S2 . Na



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (αZ)-
MF C19 H16 F2 O6 S
CI COM

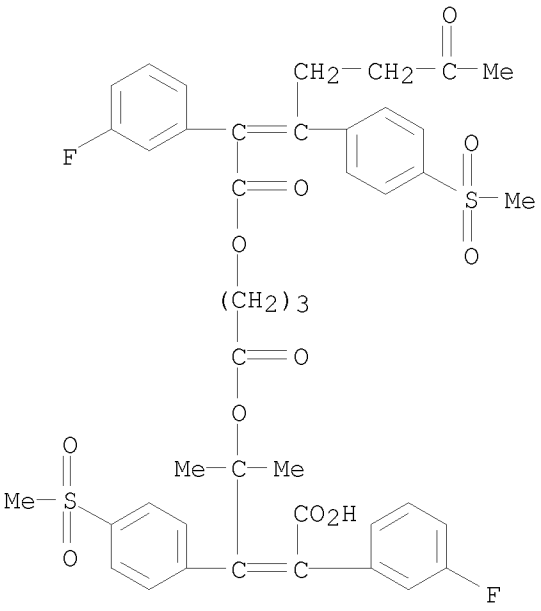
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, 3-fluoro-α-[2-[4-[[2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1,6-dioxo-2-hepten-1-yl]oxy]-1-oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-
MF C43 H42 F2 O11 S2
CI COM

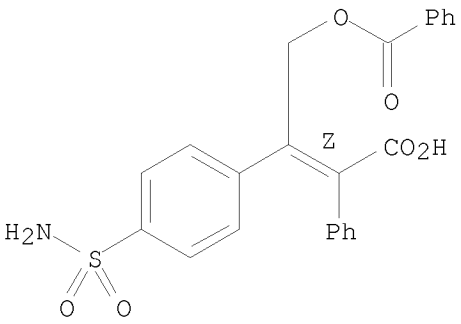


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(aminosulfonyl)phenyl]-2-(benzoyloxy)ethylidene]-, (Z)- (9CI)
MF C23 H19 N O6 S

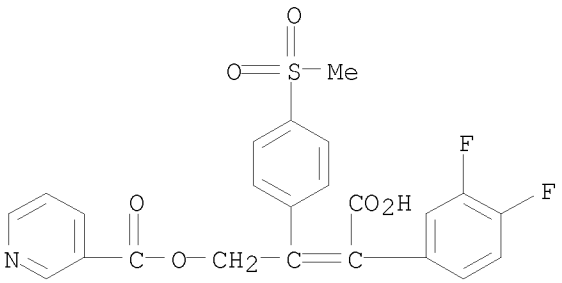
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 3-Pyridinecarboxylic acid, 3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl ester
MF C23 H17 F2 N O6 S
CI COM

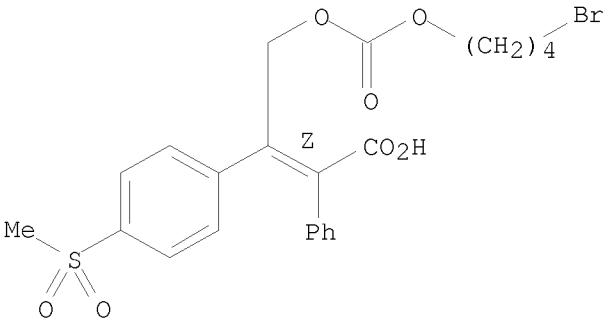


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (αZ)-
MF C22 H23 Br O7 S

Double bond geometry as shown.

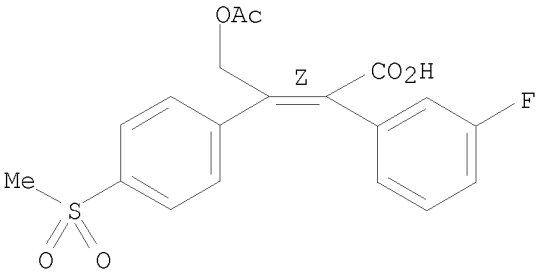


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3-fluoro-, (αZ)-
MF C19 H17 F O6 S

Double bond geometry as shown.

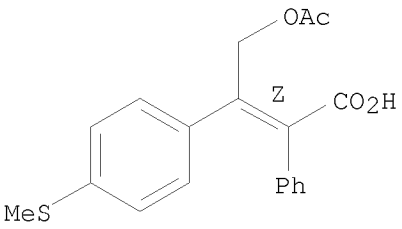


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylthio)phenyl]ethylidene]-, (αZ)-
MF C19 H18 O4 S
CI COM

Double bond geometry as shown.

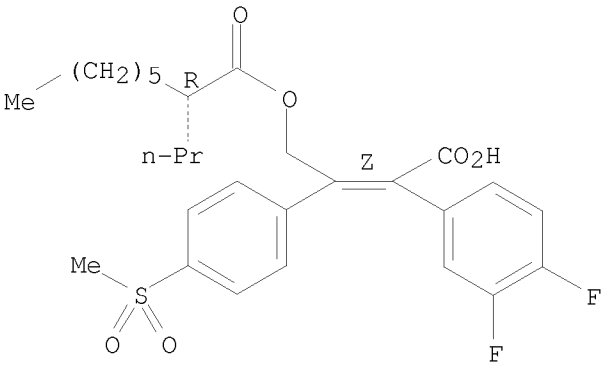


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, 3,4-difluoro-α-[1-[4-(methylsulfonyl)phenyl]-2-[[(2R)-1-oxo-2-propyloctyl]oxy]ethylidene]-, (αZ)-
MF C28 H34 F2 O6 S

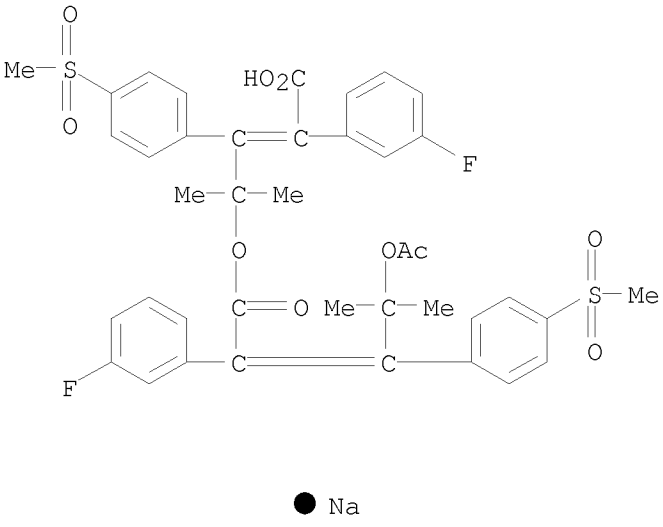
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

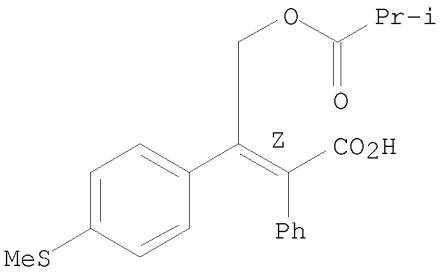
L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, sodium salt (1:1)
MF C40 H38 F2 O10 S2 . Na



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(2-methyl-1-oxopropoxy)-1-[4-(methylthio)phenyl]ethylidene]-, (αZ)-
MF C21 H22 O4 S

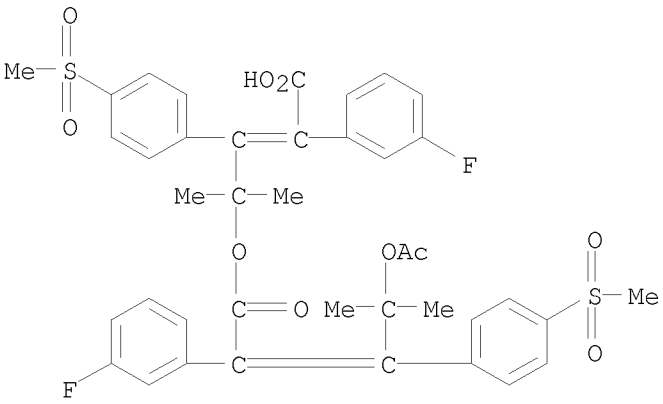
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-
MF C40 H38 F2 O10 S2
CI COM

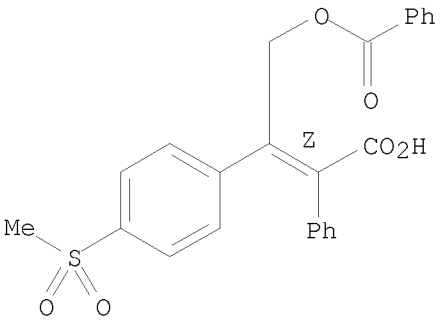


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(benzoyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (Z)- (9CI)
MF C24 H20 O6 S

Double bond geometry as shown.

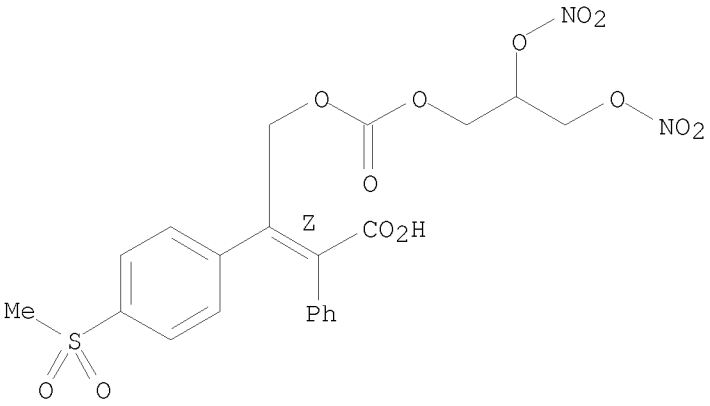


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (αZ)-
MF C21 H20 N2 O13 S

Double bond geometry as shown.

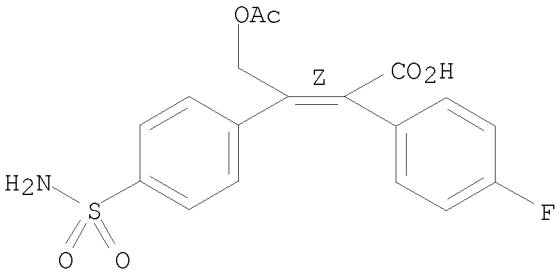


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-4-fluoro-, (Z)- (9CI)
MF C18 H16 F N O6 S

Double bond geometry as shown.

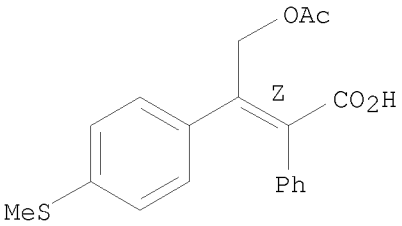


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylthio)phenyl]ethylidene]-, magnesium salt (2:1), (αZ)-
MF C19 H18 O4 S . 1/2 Mg

Double bond geometry as shown.

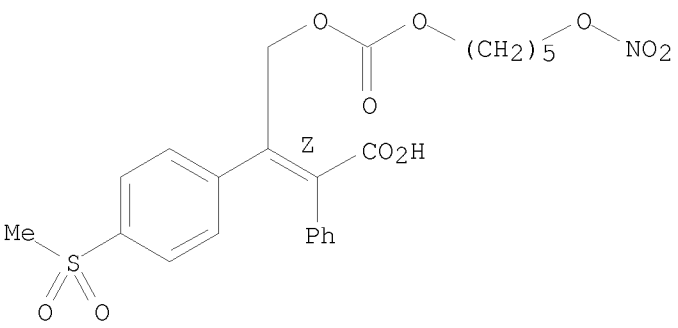


●1/2 Mg

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, (αZ)-
MF C23 H25 N O10 S

Double bond geometry as shown.

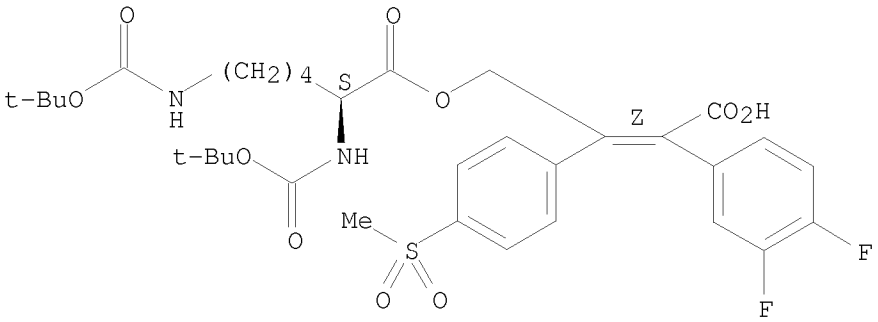


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-[[(2S)-2,6-bis[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (αZ)- (9CI)
MF C33 H42 F2 N2 O10 S

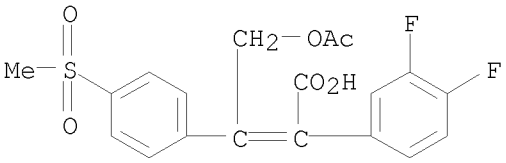
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-
MF C19 H16 F2 O6 S

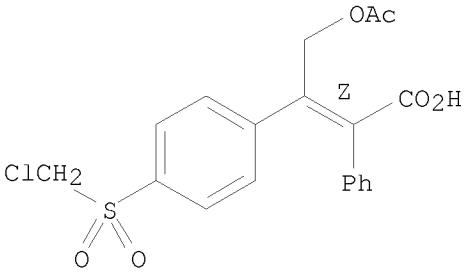


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-[(chloromethyl)sulfonyl]phenyl]ethylidene]-, (αZ)-
MF C19 H17 Cl O6 S

Double bond geometry as shown.

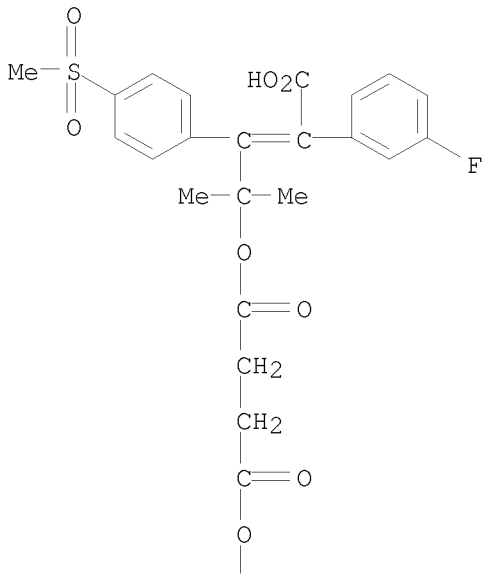


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

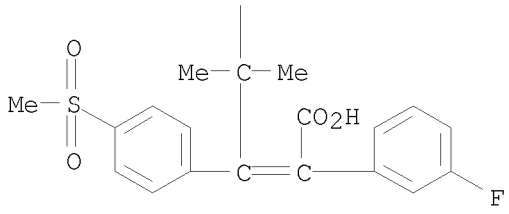
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Butanedioic acid, 1,4-bis[3-carboxy-3-(3-fluorophenyl)-1,1-dimethyl-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl] ester, sodium salt (1:2)
MF C42 H40 F2 O12 S2 . 2 Na

PAGE 1-A



PAGE 2-A

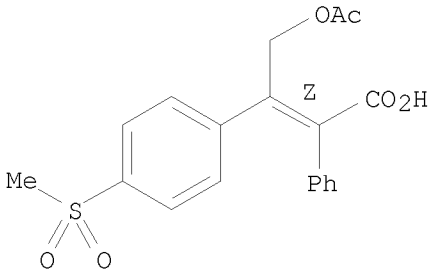


●2 Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (αZ)-
MF C19 H18 O6 S

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> 1
1 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> file zcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	190.20	190.42

FILE 'ZCAPLUS' ENTERED AT 09:46:45 ON 29 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 29 Jun 2009 VOL 151 ISS 1
FILE LAST UPDATED: 28 Jun 2009 (20090628/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

```
=> s l3
L4          15 L3

=> s l4 and (nitric (w) oxide)
         223611 NITRIC
              3 NITRICS
         223614 NITRIC
                (NITRIC OR NITRICS)
        1994871 OXIDE
         378099 OXIDES
        2101601 OXIDE
                (OXIDE OR OXIDES)
         131834 NITRIC (W) OXIDE
L5           7 L4 AND (NITRIC (W) OXIDE)

=> d sca

L5    7 ANSWERS   ZCAPLUS  COPYRIGHT 2009 ACS on STN
IC    ICM  C07C317-24
      ICS  A61K031-21
INCL 514509000; 558482000
CC    25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
      Section cross-reference(s): 1
TI    Process for making nitric oxide releasing prodrugs of
      diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors
ST    nitric oxide releasing prodrug diphenylbutenoate hexyl
      nitrate
IT    Drug delivery systems
         (prodrugs; preparation of nitric oxide releasing
         prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT    329900-75-6, Cyclooxygenase 2
      RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (inhibitors; preparation of nitric oxide releasing
         prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT    10102-43-9, Nitric oxide, biological studies
      RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (preparation of nitric oxide releasing prodrugs of
         diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT    64-19-7, Acetic acid, uses   67-68-5, Dmso, uses   68-12-2, Dmf, uses
      75-05-8, Acetonitrile, uses   75-09-2, Dichloromethane, uses   75-52-5,
      Nitromethane, uses   127-19-5, N,N-Dimethylacetamide   872-50-4,
      1-Methyl-2-pyrrolidinone, uses   1300-21-6, Dichloroethane   25321-22-6,
      Dichlorobenzene
      RL: NUU (Other use, unclassified); USES (Uses)
         (preparation of nitric oxide releasing prodrugs of
         diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT    937-14-4, m-Chloroperbenzoic acid   1504-58-1, 3-Phenyl-2-propyn-1-ol
      4286-55-9   7722-84-1, Hydrogen peroxide, reactions   10058-23-8,
      Potassium peroxymonosulfate   11138-47-9, Sodium perborate   74087-85-7,
      Dimethyldioxirane   78948-87-5, Magnesium monoperoxyphthalate
      210292-04-9, 4-Methylthiophenylmagnesium chloride
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (preparation of nitric oxide releasing prodrugs of
         diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT    176594-44-8P 179174-79-9P 754242-10-9P
      754242-11-0P   754242-12-1P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (preparation of nitric oxide releasing prodrugs of
         diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
IT    754241-98-0P
      RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
```

study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L5 7 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN
IC ICM A61K031-66
ICS A61K031-655; A61K031-21
INCL 514114000; X51-450.9; X51-415.1; X55-2 .1; X55-819.0; X55-848.2
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
TI Preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as selective cyclooxygenase-2 inhibitors
ST diarylfuranone prepn Rofecoxib prodrug nitric oxide; cyclooxygenase COX2 inhibitor diarylfuranone prepn prodrug nitric oxide
IT Pain
(chronic, treatment of; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT Anti-inflammatory agents
(nonsteroidal, medicaments with; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT Drug delivery systems
(oral; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT Analgesics
Anticoagulants
Antirheumatic agents
Combination chemotherapy
Human
(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT Drug delivery systems
(prodrugs; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT Inflammation
Osteoarthritis
Rheumatoid arthritis
Thrombosis
(treatment of; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT 50-78-2, Aspirin
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(medicaments with; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT 329900-75-6, Cyclooxygenase-2 329967-85-3, Cyclooxygenase-1
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT 754241-98-0P 754241-99-1P 754242-00-7P 754242-01-8P 754242-02-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT 108-24-7, Acetic anhydride 124-38-9, Carbondioxide, reactions 629-03-8, 1,6-Dibromohexane 1504-58-1, 3-Phenyl-2-propyn-1-ol 4286-55-9 4530-20-5, Boc-glycine 7697-37-2, Nitric acid, reactions 7722-84-1, Hydrogen peroxide, reactions 7761-88-8, Nitric acid silver(1+) salt, reactions 18162-48-6, tert-Butyl(dimethyl)silyl

chloride 162011-90-7 210292-04-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT 179174-76-6P, (2Z)-2-[4-(Methylsulfonyl)phenyl]-3-phenylbut-2-ene-1,4-diol 179174-77-7P 179174-79-9P 654068-92-5P 754242-03-0P 754242-04-1P 754242-05-2P 754242-06-3P 754242-07-4P 754242-08-5P 754242-09-6P 754242-10-9P 754242-11-0P 754242-12-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)
IT 10102-43-9, Nitric oxide, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L5 7 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN
CC 25-8 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
TI Synthesis of a NO-Releasing Prodrug of Rofecoxib
ST nitric oxide releasing prodrug of rofecoxib; stereoselective carbometalation propargyl alc
IT Metalation
(carbometalation; stereoselective synthesis of a NO-releasing prodrug of rofecoxib including carbometalation reaction of propargyl alc. derivative)
IT Stereoselective synthesis
(stereoselective synthesis of a NO-releasing prodrug of rofecoxib including carbometalation reaction of propargyl alc. derivative)
IT 100-68-5P, Thioanisole 13205-48-6P, 4-Methylthiobenzoic acid 162012-30-8P 875783-62-3P 875783-63-4P 875783-67-8P
RL: BYP (Byproduct); PREP (Preparation)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
IT 754242-04-1P
RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
IT 10102-43-9, Nitric oxide, miscellaneous
RL: MSC (Miscellaneous)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
IT 162011-90-7, Rofecoxib
RL: PNU (Preparation, unclassified)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
IT 123-09-1 1504-58-1, 3-Phenyl-2-propyn-1-ol 4286-55-9, 6-Bromo-1-hexanol 176594-44-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
IT 179174-79-9P 210292-04-9P 754242-11-0P 754242-12-1P 875783-61-2P 875783-64-5P 875783-65-6P 875783-66-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)
IT 754241-98-0P
RL: SPN (Synthetic preparation); PREP (Preparation)

```
        (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps
        from 3-phenyl-2-propyn-1-ol)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d his

     (FILE 'HOME' ENTERED AT 09:40:52 ON 29 JUN 2009)

     FILE 'REGISTRY' ENTERED AT 09:41:02 ON 29 JUN 2009
L1              STRUCTURE UPLOADED
L2            3 S SAM L1
L3           51 S FULL SSS L1

     FILE 'ZCAPLUS' ENTERED AT 09:46:45 ON 29 JUN 2009
L4           15 S L3
L5            7 S L4 AND (NITRIC (W) OXIDE)

=> exit
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                   5.80     196.22

STN INTERNATIONAL LOGOFF AT 09:48:06 ON 29 JUN 2009
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